01 SOLID FUELS

Sources, winning, properties

18/00001 Correlation of swelling and sorption properties of block coal sample

Han, F. *et al. Fuel*, 2017, 188, 452–461.

The swelling and sorption experiments were carried out simultaneously for two block coal samples under CO_2 and CH_4 pressure (up to 16 MPa) at three temperatures (25, 45 and 65 °C). The absolute sorption isotherms present type-II pattern and can be described by a modified BET model. The swelling isotherms present *L*-type pattern and can be described by a modified Langmuir model. The relationship between swelling ratio and absolute sorption amount presents *S*-type pattern and can be described by a modified Gompertz function (a logistic function). It is interesting to find that the correlations of normalized properties have a single relationship that is independent of experimental conditions, coals and gases. When the sorption amount approaches to the monolayer sorption coverage ($n_a/n_m = 1$), the swelling ratio reaches ~93% of the maximum swelling ratio. It implies the importance of the mutual contact between coal and sorbate. The differential characteristic of swelling process shows that the swelling rate with respect to sorption amount varies with the sorbate coverage; the swelling rate peaks at $n_a/n_m \approx 0.37$ and approaches zero at $n_a/n_m \approx 1.5$. In addition, a theoretical model correlating swelling and sorption was established. The concept of reduction of surface free energy by sorption was taken into account. It is encouraged that the experiment data match of model is generally acceptable.

18/00002 Depositional environment of the Lower Cretaceous Muling Formation of the Laoheishan Basin (NE China): implications from geochemical and petrological analyses

Song, Y. *et al. Organic Geochemistry*, 2017, 104, 19–34.

The Laoheishan Basin located in north-eastern China is filled with non-marine coal- and 'oil shale' (oil-prone mudstone) sediments of the Lower Cretaceous Muling Formation. Based on petrological, mineralogical and geochemical methods, the depositional environment during organic matter (OM) accumulation is investigated for the first time. The coal is subbituminous in rank. Petrological and bulk geochemical data indicate sapropelic coal, deposited in low-lying mire under freshwater conditions. High pristane/phytane ratios provide evidence for a land plant origin of OM and oxic conditions during deposition. A neutral to slightly alkaline pH is reflected by the presence of carbonate. High liptinite contents and terpenoid biomarker composition indicate high amounts of resinous OM. During 'oil shale' deposition, a raised water table was favourable for OM preservation under oxic to dysoxic conditions. The 'oil shales' in the lower unit of the succession (not associated with coal) are characterized by high hydrogen index and resinite contents interpreted to reflect deposition at elevated water depths. In contrast to the findings of previous studies on 'oil shales' in China indicating its origin from algal OM, a predominance of terrigenous OM, rich in waxy and resinous lipids, is implied from biomarker and maceral composition. The Lower Cretaceous 'oil shale' and coal in the Laoheishan Basin contain high amounts of land plant derived terpenoid biomarkers, derived from Coniferales (e.g. Pinaceae, Cupressaceae/Taxodiaceae, Araucariaceae, Podocarpaceae) and ferns. The results are in agreement with palynological data. The data highlight the potential of resinous and waxy OM to form excellent hydrocarbon source rocks.

18/00003 Dielectric properties of coal in the terahertz frequency region of 100–500 GHz

Fan, W. *et al. Fuel*, 2017, 188, 246–253.

The dielectric properties of anthracite and bituminous coals were investigated in the terahertz (THz) frequency region from 100 to 500 GHz. The authors developed two types of THz material measurement systems that can be operated in this frequency region, including one based on a vector network analyser (VNA) with frequency extension modules, and another based on a THz time-domain spectroscopy (TDS) system. Employing the free-space configuration, the authors obtained the variation of dielectric property of coals in the frequency region of 100–500 GHz. By comparing the VNA and TDS systems, the authors evaluated the continuity and consistency of the two systems and verified the dielectric property measurement results of coal in the entire frequency region. The authors first outlined the fundamental theory of dielectric property with both methods, followed by estimating the measurement error in consideration with the system stability, the time span of the time-domain gating, and measurement uncertainty. They evaluated the dielectric property of coal samples through the measured results of the VNA and TDS systems. Comparison is also made of the variation of measured dielectric property with the lower THz frequency region (W-band) in their previous work. The results show that different coal type exhibited different variation with increasing frequency in the THz band considered.

18/00004 Effects of carbon dioxide on pyrolysis of peat

Lee, J. *et al. Energy*, 2017, 120, 929–936.

This study focuses on the mechanistic understanding of effects of CO_2 on pyrolysis of peat. To do this, three pyrolytic products (i.e. syngas: H_2 and CO, pyrolytic oil (tar), and biochar) were characterized. Thermal cracking of volatile organic carbons (VOCs) generated from pyrolysis of peat was enhanced in the presence of CO_2. Besides the enhanced thermal cracking of VOCs, unknown reaction between CO_2 and VOCs was also identified. Accordingly, CO_2 played a role in enhancing syngas production and in reducing tar formation in pyrolysis of peat. This study also reveals that peat-biochar produced in CO_2 exhibited a larger surface area than that produced in N_2. The results shown in this paper would be used for various applications such as energy recovery from peat using a potent greenhouse gas (for example, CO_2).

18/00005 Properties of technological factors on screening performance of coal in an equal-thickness screen with variable amplitude

Jiang, H. *et al. Fuel*, 2017, 188, 511–521.

Screening has been widely used for the classification of particulate materials. Equal-thickness screen, which is characterized by large capacity and high efficiency, has been extensively applied in coal processing in recent years. In this paper, the method of multistage sampling and multilayer screening was used to analyse the particle size of screening products, the effects of screen surface inclination, unbalanced exciting force, excitation beam span and feed rate on the screening efficiency and partition size of coal in an equal-thickness screen with variable amplitude (VAETS) were investigated. The results showed that the sectional efficiency of the screen surface decreased along the material flow. With an increase in the screen surface length, partition size and screening efficiency gradually increased, and tended to attain a constant value. Screen surface inclination had a significant effect on partition size and screening efficiency, the partition size decreased, while the screening efficiency first increased and then decreased with an increase in the screen surface inclination. Unbalanced exciting force, excitation beam span and feed rate have a weaker impact on the partition size and screening efficiency of the VAETS. With an increase in the screen surface inclination, unbalanced exciting force, excitation beam span and feed rate, the screening efficiency first increases and then decreases. When screen surface inclination, unbalanced excitation coefficient, excitation beam span and feed rate have values of 15°, 1.228, 540 mm and 3.60 t/h, respectively, the screening efficiency reaches its maximum value of 94.37%, while the corresponding total misplaced material is 2.92%.

18/00006 Thermogravimetric and mass spectrometric (TG-MS) analysis and kinetics of coal-biomass blends

Jayaraman, K. *et al. Renewable Energy*, 2017, 101, 293–300.

In this research, thermogravimetric and mass-spectrometric (TG-MS) analysis and kinetics of coal–biomass blends (25, 50 and 75 wt%) was studied. All the experiments were performed at 20 °C/min. heating rate and under air atmosphere. The reaction regions, peak and burn-out temperatures, mass loss, maximum mass loss rate, combustion index and residue of the samples was determined. This research also focused on the main volatile products release, such as H_2, O_2, CO, CO_2 and hydrocarbons from coal-biomass blends combustion on the basis of both their relative intensities across the temperature range 150–750 °C and on their relevancy. The major release of COS is observed in decomposition stage, whereas significant SO_2 release is noticed from combustion. When the percentage of biomass is increases in the coal-biomass blends, maximum rate of mass loss increases indicating the higher reactivity of the samples. The kinetic parameters of the coal-biomass blends were calculated using two different methods (Arrhenius and Coats & Redfern). The activation energy and Arrhenius constant values were increased with the increasing biomass ratio in the blends.

Preparation

18/00007 Clean coal technology for removal dust using moving granular bed filter

Chen, Y.-S. *et al. Energy*, 2017, 120, 441–449.

An international joint research project into advanced hot gas cleaning in high-efficiency coal and solid waste power generation processes using a granular bed filter has been developed. The goal of this study is

to evaluate the filtration performance of a moving granular bed with baffle designs. A series of experiments are performed at room temperature to demonstrate the flow patterns of filtration technology (i.e. the moving granular bed filter) under different operational parameters. Pressure drops and collection efficiency are measured as performance indices and analysed through a series tests. The important parameters taken into consideration include the mass flow rates of filter granules and filtration superficial velocities. The experimental results show that the best collection efficiency is 99.87%, which is obtained using a baffle, a mass flow rate of the filter media of 600 g/min, and a filtration superficial velocity of 40 cm/s. Furthermore, the test results from this new method can be applied to moving granular bed filters or other filtration systems for a high-temperature environment of industry.

18/00008 Moisture removal mechanism of low-rank coal by hydrothermal dewatering: physicochemical property analysis and DFT calculation

Wu, J. *et al. Fuel*, 2017, 187, 242–249.

High moisture content greatly restricts the large-scale utilization of low-rank coals (LRCs). Hydrothermal dewatering (HTD) is a promising technique for dewatering and upgrading LRCs. Chinese lignite from XiMeng Mine in Inner Mongolia was upgraded by HTD. The effects of pore structure and oxygen functional group content on moisture distribution were investigated. Thermogravimetric analysis, mercury intrusion porosimetry, and chemical titration were conducted to characterize the physicochemical properties of coal samples. Results show that a substantial amount of moisture was removed, the coal composition was modified, and the energy density was significantly improved after HTD. Both free-phase and bound-phase moisture in lignite were significantly removed. Free water removal was associated with the collapse of macropore structures caused by shrinkage forces. The bound water was remarkably reduced as a result of the removal of oxygen functional groups, such as phenolic hydroxyl and carboxyl. During HTD, the oxygen functional groups were decomposed, and the hydrogen bonding between water and hydrophilic sites was destroyed, thereby leading to a weakening of the water-holding capacity of lignite. Four representative model molecules with different polarities were used to study the intermolecular interactions between lignite and water. The interaction energies of model molecule $\cdots$ water complexes were determined by density functional theory (DFT) calculation. The types of non-covalent interactions of both hydrophobic and hydrophilic sites in lignite with water were vividly demonstrated using colour-mapped reduced density gradient isosurface. The carboxyl and hydroxyl groups are extremely liable to interact with water via hydrogen bonding with large interaction energy and exhibiting strong hydrophilicity. On the other hand, the alkanes and benzene rings interact with water via van der Waals attractions and show hydrophobic effects.

18/00009 Molecular scale studies that inform trace element sulfide evaporation and atomization behavior during coal combustion

Artemyeva, A. A. *et al. Fuel*, 2017, 188, 544–552.

Understanding the chemical mechanisms of trace element (TE) evolution is essential for accurate modelling of coal combustion. A novel graphite furnace atomic absorption spectrometry (GFAAS) method was used to simulate the evaporation and atomization behaviour of TE sulfides (arsenic, antimony and selenium) in the two distinct microenvironments that mineral inclusions and exclusions experience during the onset of coal combustion. Additional insights were obtained using thermogravimetric analysis-differential scanning calorimetry (TGA-DSC). Potassium polysulfide was used as an additive to water to facilitate the dissolution of all three TE sulfides. TE sulfides in inclusions were studied by adding the test mixture to a graphite tube in a reducing (anaerobic) micro-environment whereas the TE evolution in excluded sulfide minerals was studied by blocking the graphite tube surface with an inert ZrO_2 or WO_3 coating. Arsenic sulfide, As_2S_3, exhibits a lower Arrhenius activation energy of atomization, E_a, than that of the corresponding oxide in both mineral inclusions and exclusions, apparently because of the availability of a specific facile path to atomization. A higher E_a was observed for antimony sulfide, Sb_2S_3, than that of the corresponding oxide from inclusions and is most likely due to its strong binding affinity to the carbon tube surface. The low GFAAS signal of selenium sulfide suggests the formation of molecular clusters, e.g. Se_2, Se_8 or similar mixed clusters with sulfur atoms prior to vaporization, an effect not observed for selenium oxide evaporation. For all three TE sulfides, either elemental species or unstable sulfides with low sulfur content appear to be predominant in the gas phase associated with both mineral inclusions and exclusions, with TE sulfide evaporation being the rate limiting step. Comparing the GFAAS activation energy values obtained with and without the coating showed that in a reducing micro-environment (anaerobic conditions) characteristic during the initial period of combustion for mineral inclusions, carbon merely adsorbs TE sulfides without chemical reactions. Yet TGA-DSC data showed that powdered graphite may react with TE sulfides in an oxidizing micro-environment (microaerobic conditions), such as those experienced during the later period of combustion for inclusions and during the entire combustion period for exclusions thus accelerating TE evolution without making qualitative changes in the vapour composition.

Transport, storage

18/00010 The influence of long-term storage on thermal behaviour of lower rank coal on the example of Polish coal. Part 1. The influence of long-term storage (LTS) of a lower rank coal on changes in volume of carbonized charge and changes in structural chemical parameters of pyrolysis products

Zubkova, V. *et al. Fuel*, 2017, 188, 79–89.

The pyrolysis process of a lower rank coal as a fresh coal (FC) and a long-term stored coal (LTSC) was analysed in a laboratory coking unit using X-raying and thermobalance. The changes in temperature of the charge of coals were determined along with the changes in volume of their carbonized charges, the mass loss of coals, and the mass loss rate. It was stated that LTSC has a lower thermal diffusivity at the stage of coal grain swelling and shows an almost twofold growth in charge volume at this stage. The samples of carbonized coals that correspond to the plasticity stage were investigated using the FT-IR and SEM methods. The pyrolysis products of coals were analysed by the TG/FT-IR method. It is suggested that the formation of nano-size films and spherical objects in the pores of the plastic mass of LTSC results from an increase in content of non-saturated hydrocarbons, aldehydes, phenols, and alcohols in volatile products of pyrolysis of this coal.

Economics, business, marketing, policy

18/00011 A comparative economic analysis of torrefied pellet production based on state-of-the-art pellets

Agar, D. A. *Biomass and Bioenergy*, 2017, 97, 155–161.

Torrefied pellets have fuel properties superior to those of conventional wood pellets and potentially allow greater rates of co-firing and thus larger reductions in net CO_2 emissions. Despite the growing amount of scientific output on torrefaction, the economic feasibility of torrefied pellet production is still a topic of considerable uncertainty. This is an obstacle for decision makers looking to implement sustainable energy policies. This paper compares the economics of torrefied pellets to conventional wood pellets. Working backwards from demonstrated pellet properties, this work attempts to answer the following question: Based on state-of-the-art torrefied pellets, what would be the maximum capital investment required for a torrefied pellet plant so that production is economically viable? Herein, the production costs of torrefied pellets are calculated based on inputs in production. The market value of the produced pellets is estimated and a cash-flow analysis is carried out. Three economic indicators are calculated and compared for a torrefied and conventional pellet production scenario. A sensitivity analysis is carried out for selected process inputs and the cost of CO_2 through co-firing pellets is estimated. The results indicate that state-of-the-art torrefied pellet production cannot compete with conventional pellets even with transatlantic product transport distances. A high capital investment cost and a low heating value are the main barriers to economic feasibility of state-of-the-art torrefied pellets.

18/00012 Increasing fossil power plant flexibility by integrating molten-salt thermal storage

Garbrecht, O. *et al. Energy*, 2017, 118, 876–883.

Increasing market penetration of renewable energy sources requires measures to stabilize the electric grid. This includes reducing generator output fluctuations as well as providing control reserve. The present study investigates the use of molten-salt storage systems in fossil-fired power plants by conducting a series of numerical process simulations. Two case studies are performed: First, an incinerator representing a heat-controlled facility with fluctuating output due to varying customer steam demand. Second, a small-size lignite-fired power plant for providing control reserve, representing a power-controlled facility. The results show that the concept allows significant attenuation of fluctuations in the heat-controlled facility. For a broad range of customer steam extraction, a steady production of electrical energy could be obtained without substantial modifications to the plant. Positive and negative control reserve in the power-controlled facility

can be provided through the use of a storage system with relatively low exergetic losses. However, a number of additional heat exchangers and significant modifications to the steam cycle are required.

18/00013 Switching towards coal or renewable energy? The effects of financial capital on energy transitions

Best, R. *Energy Economics*, 2017, 63, 75–83.

Does a country's stock of financial capital affect its ability to achieve energy transitions? This paper uses data for up to 137 countries for the period 1998–2013 to investigate the importance of financial capital for changes in the use of each energy type. Here the authors found that financial capital supports transition to more capital-intensive energy types. For high-income countries, financial capital facilitates transitions from fossil fuels to modern renewable energy sources, especially wind. Both private credit from banks and domestic private debt securities support greater shares of wind energy. For lower-income countries, financial capital supports progression from biomass towards fossil fuel energy sources such as coal. It was also found that countries with larger stocks of financial capital are more likely to move to more capital-intensive electricity generation systems.

Derived solid fuels

18/00014 An experimental study of ignition and combustion of single biomass pellets in air and oxy-fuel

Shan, F. *et al. Fuel*, 2017, 188, 277–284.

This study presents an experimental investigation of the ignition and combustion characteristics of single biomass pellets in air and O_2/CO_2 atmospheres containing 21%, 30%, 40%, 50% and 100% oxygen mole fractions. In this experiment, the temperature of the gas surrounding the biomass pellets was set respectively at 873, 973 and 1073 K. The rate of co-flow gas was set at 10, 15 and 20 L/min. Single pellets of *Pinus bungeana* and rice husk were fixed on a thermocouple and burned in a vertical heating tube furnace. High-speed photography was used to record images of the combustion process of biomass pellets. The resulting images exhibit two ignition behaviours: (1) homogeneous ignition of volatile, and (2) heterogeneous ignition on the particles' surface. After ignition, the combustion was no longer a homogeneous combustion of volatile. When the oxygen concentration exceeded 50%, the biomass showed a hetero-homogeneous combustion. Similarly, when the concentration of O_2 increased, the flame became shorter and more stable. With the same oxygen concentration, and once the N_2 was replaced by CO_2, the ignition delay, internal ignition temperature and the volatile combustion time increased. Inversely, when the oxygen concentration exceeded 21% (i.e. under the conditions of oxy-fuel), these parameters were correspondingly reduced. In other words, the ignition and combustion intensity were increased. The effects of oxygen concentration and co-flow temperature on ignition and combustion of biomass pellets were greater than that of co-flow velocity. The study's results show that the biomass pellets did not break during combustion.

18/00015 Anode coke from coal – a low cost approach

Craddock, J. D. *et al. Fuel*, 2017, 187, 229–241.

Declining quality and availability of petroleum cokes, which have traditionally been used for the production of carbon anodes, is forcing aluminium producers to use cokes previously regarded as unsuitable. Domestic reserves of coal represent a potential alternative carbon resource for anode production, provided coke specifications can be economically achieved. Previous studies have shown that the solvent refining of coal could produce carbons suitable for aluminium production. To conform to coke specifications (e.g. metals content), it was necessary to remove mineral matter in the coal by a costly filtration step. This adds significantly to the cost of the process, making it uncompetitive with coke from other sources. However, cokes with properties very similar to the required specifications have been produced from very low ash coals by solvent extraction, but without the uneconomic solids removal step. Extraction in a suitable solvent was used to produce a coal digest, which when injected at high temperature into a coking vessel generated the anisotropic needle structure characteristic of high quality cokes. Reported here are the results of this investigation into using low-ash coals (1–2 wt%) from the south-eastern Kentucky coalfield to produce anode-grade cokes using similar methods. The high cost filtration step was omitted, but the resulting coke did not meet the anode grade specifications.

18/00016 Effect of catalysts on char structural evolution during hydrogasification under high pressure

Liu, X. *et al. Fuel*, 2017, 188, 474–482.

The catalytic hydrogasification of coal char was investigated in a high-pressure fixed-bed tube reactor using CaO, $CaCO_3$, Na_2CO_3 and K_2CO_3 as catalysts. Experimental results showed that the char reactivity could be greatly improved with the addition of catalysts. Analysis of char structural evolution was performed to further explore the catalytic mechanism by employing Raman spectroscopy and scanning electron microscopy combined with energy dispersive X-ray spectroscopy (SEM-EDX). The results revealed that CaO catalyst inhibited the aromatic ring condensation of the char structure during hydrogasification. The catalytic reaction of CaO only occurred on the char surface. Na_2CO_3 or K_2CO_3 was reduced to metallic Na or K and diffused into the char under hydrogen atmosphere, enhancing the cracking of large aromatic ring systems into small ones, which were the active species for hydrogasification. The catalytic reaction of alkali catalyst occurred simultaneously on the surface of and inside the char. Therefore, the Na_2CO_3 and K_2CO_3 displayed higher catalytic activities than CaO in hydrogasification.

18/00017 Influence of AAEM species in coal and biomass on steam co-gasification of chars of blended coal and biomass

Zhang, Z. *et al. Renewable Energy*, 2017, 101, 356–363.

This study investigated effects of blending ratio and alkali and alkaline earth metallic (AAEM) species in the feedstock on char reactivity and producer gas composition in steam co-gasification of chars of blended coal and biomass. Experiments were conducted on a bench-scale fixed bed gasifier in which lignite was used as coal and radiata pine was used as biomass. The blending ratios of lignite to pine (L/P) were, respectively, 0 : 100 (pure pine), 20 : 80, 50 : 50, 80 : 20 and 100 : 0 (pure lignite). Lignite and radiata pine were first separately ground to fine particles which were then blended based on pre-set ratios. After this, the blends were pelletized and charred at 900 °C. In order to investigate the effect of AAEM in the coal, experiments were also performed using blended pine and acid-washed lignite from which most of AAEM species were effectively removed. The co-gasification operation temperature was 950 °C. From the experimental results, it was found that the ratios of H_2/CO, H_2/CO_2 and CO/CO_2 in the producer gas were non-linearly related to L/P ratio in the lignite blended chars; however, these gaseous ratios were linearly correlated to the L/P ratio in co-gasification of acid-washed lignite blended chars. In addition, by removing the AAEM species in lignite, yields of H_2 and CO_2 were reduced while CO yield was increased. The char reactivity of acid-washed lignite and pine blends was decreased and this decrease became more significant with increase in coal to biomass blending ratio.

18/00018 Study of the transient combustion of highly densified biomass briquette (Bio-coke) in an air flow

Yan, H. and Fujita, O. *Fuel*, 2017, 188, 595–602.

End-face combustion experiments were conducted on cylindrical bio-coke (BIC), i.e. a highly densified biomass briquette, to investigate whether quasi-one-dimensional steady combustion can be attained in 400 K air flow, as measured by a steady regression rate. In the experiment, it was found that the average regression rate in the first 0.01 m of BIC was relatively small after ignition, whereas after the first 0.01 m, the average regression rate became almost steady and much larger than that in the first 0.01 m. This suggests that before the steady regression period is reached, a non-negligible unstable regression rate phase exists. To investigate this transient combustion phase, one-dimensional numerical calculations were conducted, and the time-dependent regression rate and temperature distribution were computed. The mechanisms controlling transient combustion and the effects of volatile and moisture contents on transient combustion behaviour were examined. The results show that a transient combustion period exists before steady combustion is achieved. This transient combustion period decreases as volatile content increases, and moisture content has a similar effect on transient combustion as volatile content. The phenomenon can be explained by the different final steady temperature distribution and evolution rate from the initial temperature distribution to the final steady temperature distribution.

18/00019 Theoretically designed metal-welded carbon nanotubes: extraordinary electronic properties and promoted catalytic performance

Liao, T. *et al. Nano Energy*, 2017, 32, 209–215.

The properties of either carbon nanotubes (CNTs) or nanoribbons (CNRs) in their pristine form are nevertheless insufficient to satisfy the increasing demands of various applications. Strategies that can endow these carbon-based nanostructures with guided functionalization are in urgent need. This study theoretically demonstrates that carbon nanoribbons can be welded by a variety of metal-atoms, such as alkali metals, III–IV group metals, and transition-metals, to form functionalized metal-welded carbon nanotubes (MW-CNTs), which represent a new family of carbon-based nanostructures. It is significant that the metal-welded CNTs exhibit noticeably lower formation energies than their nanoribbon counterparts, indicating that this new family of carbon nanostructures can be synthesized experimentally. The introduction of the hetero-metal-atoms endows MW-CNTs with fascinating

tailored properties. For example, in the 3*d* magnetic transition-metal-welded (Cr, Mn and Fe) nanotubes, Cr-welded CNTs show half-metallic properties, giving them potential applications in spintronic or magnetic devices; while Fe-welded CNTs display superior catalytic activity towards the dissociation of water molecules. The salient electronic and catalytic properties of this novel family of metal-welded carbon nanotubes pave the way to design high-performance devices for energy harvesting, conversion and storage. More importantly, the idea of heteroatom welding of foldable two-dimensional systems may develop into a versatile design strategy that can be extended to BN, MoS_2, TiO_2, and other two-dimensional (2D) nanosheets.

02 LIQUID FUELS

Sources, properties, recovery

18/00020 Accurate determination of bubble-point of oils from *PV* data using a combination of *Y*-function and Tait equation

Hoang, H. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 801–810.

This work provides a numerical approach, relying on robust fluid models, to estimate accurately the bubble point of oils from pressure-volume data. The proposed scheme relies on the Tait equation to accurately model the liquid data and on the efficiency on the Y-function to describe the two-phase data. This operator independent scheme has been applied to a set a black-oils and volatile oils of reliable literature experimental data. Results show that the proposed scheme yields bubble-point pressures with deviations of a few psi when compared to experiments. More precisely, an average absolute deviation smaller than 0.3% was obtained, which is one order of magnitude better than usual approaches.

18/00021 An efficient geometry-based optimization approach for well placement in oil fields

Hamida, Z. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 383–392.

This study aims at introducing a problem-specific modified genetic algorithm (GA) approach for optimal well placement in oil fields. The evolution method used in this algorithm includes a novel genetic operator named 'Similarity Operator' alongside the standard operators (i.e. mutation and crossover). The role of the proposed operator is to find promising solutions that share similar features with the current elite solution in the population. For the well placement problem in oil fields, these features include the new well location with respect to pre-located wells and the porosity value at the proposed location. The presented approach highlights the importance of the interaction between the nominated location and the pre-located wells in the reservoir. In addition, it enables systematic improvements on the solution while preserving the exploration and exploitation properties of the stochastic search algorithm. The robustness of genetic similarity algorithm is assessed on both the PUNQ-S3 and the Brugge field data sets.

18/00022 Controls on reservoir quality in exhumed basins – an example from the Ordovician sandstone, Illizi Basin, Algeria

English, K. L. *et al. Marine and Petroleum Geology*, 2017, 80, 203–227.

Petroleum exploration in many North African intracratonic basins targets Early Paleozoic sandstones as the primary reservoir objective. These sandstones are often characterized by highly variable reservoir quality (0.0001–1000 mD), and the ability to predict and selectively target areas of enhanced porosity and permeability is crucial to unlock the hydrocarbon potential. The objective of this study is to characterize the primary controls on reservoir quality in an Ordovician field in the Illizi Basin of Algeria through detailed core and petrographic analysis, and establish if variations in thermal history across the field have a material impact on reservoir quality. The best reservoir quality is observed in facies where primary intergranular porosity has been preserved in fine to coarse-grained quartzarenites with less than 1% fibrous illite. These lithologies are most commonly found within the high-energy, tidally reworked, post-glacial facies sandstones of the uppermost Ordovician succession. Observed differences in quartz cement volume within compositionally and texturally similar samples from the southern and northern parts of the field are interpreted to reflect variations in thermal exposure due to deeper burial. This interpretation is supported by field-wide numerical modelling of sandstone diagenesis. This study indicates that subtle variations in thermal history can have a material impact on the spatial trends in reservoir permeability. Thermal history, therefore, is an important consideration in reservoir quality studies in exhumed basins where variations in present-day burial depth will be a poor guide for evaluating reservoir quality risk across a basin or play.

18/00023 Density, viscosity and specific heat capacity of diesel blends with rapeseed and soybean oil methyl ester

Giuliano Albo, P. A. *et al. Biomass and Bioenergy*, 2017, 96, 87–95.

By 2020, the EU aims to have 10% of the transport fuel of every EU countries come from renewable sources such as biofuels. Fuel suppliers are also required to reduce the greenhouse gas intensity of the EU fuel mix by 6% in comparison to 2010. The thermophysical properties of biofuels are, therefore, required for the efficient design of every step in their production, distribution, and utilization. Despite of these needs, high pressure thermodynamical characterization of biofuels is not still exhaustive. Next generation injection systems work with pressure up to 300 MPa, but available measurements are limited to 200 MPa. Measurements extrapolation generally are not recommended at these pressure because it can hide freezing phenomena here documented at temperature of (20 and 30) °C. In this work, density and viscosity of pure and blended FAME (SME and RME) biofuels have been measured up to 300 MPa. Since the scope of the work is both to investigate cold start conditions found in engines and the thermal behaviour of fuels in tanks of cars, petrol station and dispenser, the temperature interval is limited to (0–60) °C. In particular, it has been observed a partial freezing even for temperature up to 30 °C. Density and viscosity values were obtained by direct experimental measurements, while heat capacities have been calculated using density and speed of sound results previously obtained. At ambient pressure conditions, the uncertainty in density measurements was between 0.005% and 0.01% ($k = 2$) and for viscosity measurements the uncertainty was between 0.2% and 1.3% ($k = 2$). At elevated pressures the uncertainty in density measurements was 0.08% ($k = 2$), while for viscosity and heat capacity it was 2% ($k = 2$).

18/00024 Development and validation of an explicitly coupled geomechanics module for a compositional reservoir simulator

Haddad, M. and Sepehrnoori, K. *Journal of Petroleum Science and Engineering*, 2017, 149, 281–291.

Pore pressure-stress analyses in stress-sensitive reservoirs investigate interactions between the *in situ* stress and fluid flow; these interactions help or resist production, or conclude surface subsidence during production. Among the tools for these analyses, an explicitly coupled geomechanics and fluid flow model provides an essential, reliable, and fast production estimate for field planning and development. This work implements the model in an in-house, three dimensional, compositional reservoir simulator, UTCOMP, using Chin's iterative coupling method. This development integrated a stand-alone geomechanics module based on finite element method with the reservoir simulator, an advantage of this coupling algorithm, and improved the understanding of the production through various enhanced oil recovery processes such as water and CO_2 flooding processes previously coded in UTCOMP. Benefiting from the higher time scales of solution variations due to the geomechanics module, the authors lowered the frequency of calling this computationally expensive module. Also, they reduced the order of the finite element shape functions for displacement from quadratic to linear, which majorly mitigated the high computational cost of the geomechanics studies while the solution accuracy was almost maintained. To validate the implementation, the authors investigated a primary oil production case and compared the results from UTCOMP with those from two other simulators: (1) CMG software program using different coupling methods; and (2) another pre-validated in-house reservoir simulator, GPAS. In order to evaluate the improvements in this work, the results were compared with those from a pre-validated in-house reservoir simulator, GPAS. A minor discrepancy was observed between the solutions at very early times which originates from the different structures in these two reservoir simulators, IMPEC in UTCOMP and fully implicit in GPAS.

18/00025 Energy analysis of oil-water flow with drag-reducing polymer in different pipe inclinations and diameters

Al-Wahaibi, T. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 315–321.

In this study, the energy analysis of oil-water flow with polymer additives in terms of the reduction in head loss, which results in reducing the pumping power required to overcome the head loss and in turn increasing the throughput was carried out. Three acrylic pipes with internal diameters of 30.6, 55.7 and 74.7 mm were used in the study. The 30.6-mm ID pipe was positioned at horizontal (0°), upward (+5° and +10°) and downward (−5°) inclinations while the 55.7-mm and 74.7-mm ID pipes were only at horizontal position. The oil–water

flow conditions of 0.4–1.6 m/s mixture velocities and 0.1–0.9 input oil volume fractions were used. Master solution of 2000 ppm concentration of water-soluble polymer – a high-molecular-weight anionic copolymer of polyacrylamide and 2-acrylamido-2-methylpropane sulfonic acid – was prepared and injected at controlled flow rates to provide 40 ppm of the polymer in the water phase at the test section. It was found that the presence of the polymer positively influenced the three parameters investigated. Specifically, the head loss was reduced from 0.0885 to 0.0378 m, translating to a saving of 57.3% in pumping power requirement and 61% increase in the throughput at a flow condition in the 30.6-mm ID pipe where the performance of the polymer was highest.

18/00026 Generalized sensitivity analysis study in basin and petroleum system modeling, case study on Piceance Basin, Colorado

Tong, Y. and Mukerji, T. *Journal of Petroleum Science and Engineering*, 2017, 149, 772–781.

Basin and petroleum system modelling is an interdisciplinary endeavour, and utilizes integrated data to study sedimentary basins. Numerical models are constructed and simulated to quantitatively model the geodynamic processes in sedimentary basins. Often, the modelling process covers large spatial and temporal intervals with many uncertain input parameters. These can be continuous parameters characterized by certain statistical distribution, spatially distributed variables, or discrete parameters such as geological scenarios. Identifying sensitivities from these complex input model parameters and recognizing key uncertainties are crucial and challenging for basin modelling development and applications. The major contribution of this work is to introduce and implement efficient and accurate sensitivity analysis approach for basin and petroleum system modelling discipline. The authors investigated two types of sensitivity analysis methods and compared their performance for identifying the impact of uncertain parameters on both spatial and temporal model responses. The first approach utilizes the variance-based Sobol indices to quantify parameter sensitivities, while the second approach is a distance-based sensitivity analysis which utilizes the distance between model responses to determine sensitivities of different parameters. The sensitivity analysis approaches are illustrated through a basin modelling example involving the processes of sediment compaction, source rock maturation and hydrocarbon generation in the Piceance Basin, Colorado, US. Monte Carlo samples of the input uncertainties related to physical properties of the source rock, thermal boundary conditions, and geological setting scenarios are generated. Multiple basin models constructed using these uncertain input parameters are simulated across the geological time span, and time-varying model response (hydrocarbon generation from Lower Cretaceous to present-day) and spatial model response (pressure and porosity distribution at present-day) are obtained. Sensitive parameters that impact these spatio-temporal model responses are then analysed. Results show that the distance-based sensitivity analysis approach could achieve similar results with fewer model runs compared to the variance-based Sobol method. Model responses in spatial and temporal domain are impacted by different uncertain input parameters. Subtle relationship between input parameters and model response could also be identified. In particular an unexpected link between chemical kinetics and porosity versus depth behaviour was uncovered. The knowledge obtained from sensitivity studies enhance the understanding of the complex geological processes and can benefit the modelling development and forecast capability. Though the sensitivity results are case-specific, the approach and workflow are generally applicable to other basins and earth sciences modelling studies.

18/00027 Geochemistry and charge history of oils from the Yuqi area of Tarim Basin, NW China

Song, D. *et al. Marine and Petroleum Geology*, 2017, 79, 81–98.

The geochemistry, origin and charge history of oils from the Yuqi area of Tarim Basin have been investigated, through GC, GC-MS and fluid inclusion microthermometry analysis. The Yuqi oils accumulated mainly in three intervals: (1) in the Lower-Middle Ordovician Yingshan Formation ($O_{1-2}y$) carbonate reservoirs; (2) in the overlying Upper Triassic Halahatang Formation (T_3h) and (3) in the Lower Cretaceous Yageliemu Formation (K_1y) sandstones. Oils from different reservoirs have distinct physical properties, varying from extra-heavy ($O_{1-2}y$), heavy (T_3h), to light oils (T_3h and K_1y). However, their geochemical compositions show a high degree of similarity, which indicates that they derive from the same source rock. Abundant tricyclic terpanes, gammacerane, dibenzothiophene and C_{21}–C_{22} steranes, together with a low level of diasteranes, indicate an anoxic marine source rock for oils in the Yuqi area. Oil–oil correlation shows that Yuqi oils derive from the same source bed as Tahe oils. The co-occurrence of intact *n*-alkanes and 25-norhopanes in all the samples supports the proposition that there is a mixture of an early filled severely biodegraded oil and a late filled fresh oil. In this study, charge history is examined on the basis of integration of fluid inclusion homogenization temperature data with 1D burial-thermal history models. Two episodes of oil charging are identified in the $O_{1-2}y$ reservoir (well YQX1-1) at around 436–420 Ma (Middle-Late Silurian) and 10–3 Ma (Miocene to Pliocene), respectively. For the samples from the T_3h and K_1y intervals, only one episode of oil charge is indicated by the homogenization temperatures of coexisting aqueous inclusions with an inferred timing around 10–3 Ma. The T_3h heavy oil reservoir is assumed to be a secondary hydrocarbon pool, which accumulated by re-migration and re-distribution of hydrocarbons from $O_{1-2}y$ hydrocarbon pools. The few early biodegraded oils in the K_1y light oils were probably picked up along the migration pathway during the late fresh oil charging.

18/00028 Hydrocarbon expulsion potential of source rocks and its influence on the distribution of lacustrine tight oil reservoir, Middle Permian Lucaogou Formation, Jimsar Sag, Junggar Basin, Northwest China

Bai, H. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 740–755.

The petroliferous Permian system of the Junggar Basin in northwest China is predominantly a conventional oil exploration region. To assist in the unconventional tight oil reservoir exploration, the hydrocarbon expulsion potential of source rocks and its influence on the tight oil distribution of the Middle Permian Lucaogou Formation (P_2l) in the Jimsar Sag are discussed. The research is based on geological and geochemical characteristics such as the distribution, abundance, type, thermal maturity of source rocks, and 'sweet spots'. Meanwhile, hydrocarbon expulsion intensity and quantity were evaluated with hydrocarbon generation potential method. The Middle Permian Lucaogou source rocks have wide distribution and high thickness (mostly thicker than 100 m). The source rocks exhibit low to high TOC (mainly ranges from 1.0 to 5.0 wt%) and primarily contain type-II kerogen, resulting in significant hydrocarbon expulsion potential under moderate mature thermal evolution (R_o mainly ranges from 0.55% to 1.05%). According to the hydrocarbon expulsion modelling, the source rocks reached the hydrocarbon expulsion threshold at 0.73% R_o and the hydrocarbon expulsion rate became greatest at 0.9% R_o. The comprehensive hydrocarbon expulsion efficiency was approximately 48%. About 18.7×10^8 t of hydrocarbons were expulsed from the Lucaogou source rocks in the Jimsar Sag. The hydrocarbon expulsion intensities are relatively large and range from 150×10^4 t/km^2 to 400×10^4 t/km^2 in the centre and west area of the sag, where is the superimposed area of source rock thicker than 200 m, TOC greater than 3.5% and R_o higher than 0.85% in the sag. There are 17 exploratory wells obtaining commercial oil flow in the sag. Sixteen of the 17 exploratory wells are located in the area with hydrocarbon expulsion intensity greater than 50×10^4 t/km^2. By contrast, other exploratory wells outside the hydrocarbon expulsion coverage area have slight show of oil, even dry. In addition, there is positive correlation between the hydrocarbon expulsion intensity and the daily output of well testing. It is concluded that the tight oil exploration should focus on the area with hydrocarbon expulsion intensity greater than 100×10^4 t/km^2, which is a favourable area for commercial hydrocarbon accumulation and exploration.

18/00029 Hydrocarbon source rock potential in the southwestern Gulf of Suez graben: insights from organic geochemistry and palynofacies studies on well samples from the Ras El Bahar Oilfield

El Diasty, W. S. *et al. Marine and Petroleum Geology*, 2017, 80, 133–153.

Palynological and biomarker characteristics of organic facies recovered from Cretaceous–Miocene well samples in the Ras El Bahar Oilfield, southwest Gulf of Suez, and their correlation with lithologies, environments of deposition and thermal maturity have provided a sound basis for determining their source potential for hydrocarbons. In addition to palynofacies analysis, TOC/Rock-Eval pyrolysis, kerogen concentrates, bitumen extraction, carbon isotopes and saturated and aromatic biomarkers enable qualitative and quantitative assessments of sedimentary organic matter to be made. The results obtained from Rock-Eval pyrolysis and molecular biomarker data indicate that most of the samples come from horizons that have fair to good hydrocarbon generation potential in the study area. The Upper Cretaceous–Paleocene–Lower Eocene samples contain mostly Type-II to Type-III organic matter with the capability of generating oil and gas. The sediments concerned accumulated in dysoxic–anoxic marine environments. By contrast, the Miocene rocks yielded mainly Type-III and Type-II/III organic matter with mainly gas-generating potential. These rocks reflect deposition in a marine environment into which there was significant terrigenous input. Three palynofacies types have been recognized. The first (A) consists of Type-III gas-prone kerogen and is typical of the Early–Middle Miocene Belayim, Kareem and upper Rudeis formations. The second (B) has mixed oil and gas features and characterizes the remainder of the Rudeis Formation. The third association (C) is dominated by amorphous organic matter, classified

as borderline Type-II oil-prone kerogen, and is typical of the Matulla (Turonian–Santonian) and Wata (Turonian) formations. Rock-Eval T_{max}, PI, hopane and sterane biomarkers consistently indicate an immature to early mature stage of thermal maturity for the whole of the studied succession.

18/00030 In situ stress field evaluation of deep marine tight sandstone oil reservoir: a case study of Silurian strata in northern Tazhong area, Tarim Basin, NW China

Yin, S. *et al. Marine and Petroleum Geology*, 2017, 80, 49–69.

Deep marine tight sandstone oil reservoirs are the subject of considerable research around the world. This type of reservoir is difficult to develop due to its low porosity, low permeability, strong heterogeneity and anisotropy. A marine tight sandstone oil reservoir is present in the Silurian strata in the northern Tazhong area of the Tarim Basin, north-west China, at a depth of more than 5000 m. The porosity is between 6% and 8%, and the gas permeability is between 0.1 and 1×10^{-3} μm^2. The features of this type of reservoir include the poor effects of conventional fracturing modifications and horizontal wells, which can lead to stable and low levels of production after staged fracturing. A comprehensive evaluation of the mechanical properties of the rock and the *in situ* stress of the target tight sandstones was conducted by using numerous mechanical and acoustic property tests, conducing crustal stress analysis and using data from thin section observations. The dispersion correction technique is used to transform velocity at the experimental high frequency (1 MHz) to velocity at the logging frequency (20 kHz). The logging interpretation models of the transverse wave offset time, mechanical parameters and *in situ* stress are calculated, and each model represents a high precision prediction. Simulating the *in situ* stress field of the Silurian strata using a three-dimensional finite element method demonstrates that the average error between the simulation result and the measured value is less than 6%. The planar distribution of each principal stress is mainly controlled by the burial depth and fault distribution. By conducting *in situ* stress orientation analysis for the target layer via the analysis of paleomagnetism, borehole enlargement, fast shear wave orientation and stress field simulation, it was shown that the direction of the maximum horizontal stress is N45E. In this paper, a typical and successful comprehensive evaluation of the stress field of the deep tight sandstone oil reservoir is provided.

18/00031 Linking fluid composition to black-oil properties

Mogensen, K. *Journal of Petroleum Science and Engineering*, 2017, 149, 161–170.

Field development studies require, among many other things, reliable estimates of fluid properties. In cases where experimental data are unavailable or incomplete, it is necessary to predict fluid properties using correlations, based on input variables such as temperature, API, saturation pressure, gas gravity, and flash GOR. However, there are situations when even these input variables are not known, and where the only information is the initial reservoir fluid composition. The scope of the present work is to develop a predictive method which links the reservoir fluid composition to the input variables needed for the black-oil property correlations. The method is based on analysis of several experimental data sets comprising in total several hundred fluid compositions with associated black-oil properties as well as on isothermal flash calculations on 500,000 synthetic, but realistic, fluid compositions spanning a large range in compositional space. The aim of this work is therefore not to develop new correlations for oil compressibility, formation volume factors, viscosities etc. Rather, the contribution should be regarded as a novel way to incorporate reservoir fluid compositional information into an already existing framework for predicting fluid properties used for field development studies. Results from the study show that it is possible to predict API, flash gas gravity, flash GOR and saturation pressure with reasonable accuracy for a large range of reservoir fluid compositions as long as the molecular weight of the plus fraction is known. The work sheds more light on the quantitative influence of individual component mole fractions on fluid properties.

18/00032 Linking the Acadian Orogeny with organic-rich black shale deposition: evidence from the Marcellus Shale

Chen, R. and Sharmal, S. *Marine and Petroleum Geology*, 2017, 79, 149–158.

The trace and rare earth elements (REE) analyses were conducted on samples collected from a 30 m core of the Marcellus Shale obtained from Greene County, south-western Pennsylvania, USA. The results suggest that organic matter enrichment trends in the Marcellus Shale can be directly linked with the Acadian Orogeny. The Acadian Orogeny has been recognized as a main sediment source for the Marcellus Shale. Synthesis of tectonic history and recent ash bed geochronology, reveals that deposition of the organic carbon-rich (OR) zone (characterized by TOC > 4%; located between 2393 and 2406.5 m core depth) in the studied Marcellus Shale core was coincident with tectonically active and magmatic quiescent period of the Acadian orogeny (*ca*. 395–380 Ma). This time period also corresponds to the highest rate of mountain building in the Acadian Orogeny. The light rare earth (LREE) and selected trace elemental (e.g. Ta, Cs) composition of the OR zone sediments is similar to that of the bulk continental crust, supporting the lack of magmatic activity in the source area (i.e. Acadian Orogeny). In contrast, subsequent deposition of the organic carbon-poor (OP) sediments (characterized by TOC < 4%; located between 2376 m and 2393 m core depth) in the upper Marcellus Shale occurred synchronously with a magmatic active phase (*ca*. 380–370 Ma) during the Acadian Orogeny. The OP zone sediments have LREE and trace elemental composition similar to the average of the upper continental crust, suggesting intrusion of granodiorite rocks during a magmatic active period of Acadian Orogeny. The temporal and geochemical correlation between the Acadian orogenesis and the Marcellus deposition provide evidence for the role of tectonism in the enrichment of organic matter in the Marcellus Shale.

18/00033 Methods for determining asphaltene stability in crude oils

Guzmán, R. *et al. Fuel*, 2017, 188, 530–543.

Different tests used to predict asphaltene stability in crude oils, such as colloidal instability index, colloidal stability index, Stankiewicz plot, qualitative-quantitative analysis, stability cross plot, Heithaus parameter, toluene equivalence, Bureau of Mines correlation index – toluene equivalence, and oil compatibility model are reported in this work. In addition, SARA fractionation, asphaltene flocculation point, P-value, S-value, separability number, stationary column stability test, compatibility test, and spot test are disclosed. Using experimental data reported in literature, each test is carried out in order to evaluate its accuracy finding that some tests predict the asphaltene stability better than other ones. It was found that qualitative-quantitative analysis and stability cross plot behaved better than colloidal instability index and Stankiewicz plot.

18/00034 Multi-element analysis of crude oils using ICP-QQQ-MS

Walkner, C. *et al. Organic Geochemistry*, 2017, 103, 22–30.

Determination of trace element contents in crude oils constitutes a powerful geochemical tool, complementing organic geochemical analyses and allowing a deeper insight into the processes of oil generation, migration and maturation. Inductively coupled plasma mass spectrometry (ICP-MS) has been widely applied to trace element determination in petroleum samples due to its low detection limits and fast multi-element capability. However, quantification of several elements by quadrupole-based ICP-MS is hampered by low sensitivity due to high ionization energy, severe polyatomic interferences and/or low abundance. In the present contribution an ICP tandem mass spectrometer (ICP-MS/MS), or triple quadrupole ICP-MS (ICP-QQQ-MS) has been used to overcome these limitations. Prior to analysis, samples were subjected to high pressure acid digestion, allowing external calibration by means of aqueous standards. 25 elements, including P, S, the first-row transition metals, As, Se, Re, Pb and U, could be quantified in one measurement. Polyatomic interferences on the lighter elements could be removed by reaction of the target ions with O_2 or NH_3 in the collision/reaction cell of the ICP-MS/MS. The accuracy of the analytical method was assessed by the analysis of the standard reference materials NIST SRM 1634c (trace elements in fuel oil) and 1084a (wear-metals in lubricating oil). The measurement procedure was applied to the analysis of crude oil samples from the Alpine Foreland Basin of Austria.

18/00035 Multi-technique approach to the petrophysical characterization of Berea sandstone core plugs (Cleveland Quarries, USA)

Kareem, R. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 436–455.

Berea sandstone has been used by the petroleum industry as a representative model siliciclastic rock for a number of years. However, only incomplete data has been reported in the literature regarding its petrographic, geochemical, and petrophysical properties. In particular knowledge of the mineral distribution along the pore walls is particularly scarce, despite the fact that mineral exposed in the pore space will be crucial in determining the rock-fluid interactions that occur during core-flooding experiments. In this paper, four Berea sandstone samples (with four different permeability ranges from <50, 50–100, 100–200 and 500–1000 mD) were subjected to a multi-technique characterization with an emphasis on determining the mineral composition, and distribution at the pore surface as well as pore structure and connectivity analysis. The mineral distribution was measured in two-dimensions by chemical mapping using energy dispersive X-ray spectroscopy–scanning electron microscopy (SEM–EDX). The bulk composition of the Berea sandstones was also measured by X-ray diffraction and micro-X-ray computed tomography. From this, it was found that authigenic minerals, especially clay minerals, make up a small portion of the bulk rock volume (3.3–8%)

but are over-represented at the pore surfaces and in pore spaces compared to the other major mineral constituents of the rock (quartz and feldspar). The effective mineralogy, from the standpoint of rock-fluid interactions, is the mineralogy that predominates at pore surfaces. For the Berea sandstone samples studied, the effective mineralogy is represented, mainly, by kaolinite, illite, and chlorite. For three of the four permeability ranges studied, kaolinite is the predominant pore lining mineral observed. In the remaining sample (50–100 mD), illite is the predominant mineral. In addition to SEM, the authors used atomic force microscopy to show that the nano-sized particles with the shape and size of clay crystals are observed on the surface of recrystallized quartz grains in a Berea sample. Regardless of their origin and identity, the presence of these particles shows that the quartz grain surfaces in Berea sandstone are more heterogeneous than previously assumed. Carbonate cement was somewhat localized throughout two of the Berea sandstone specimens, however, quartz cement is common in all of the Berea cores studied and include both microcrystalline quartz and amorphous silica phases. The pore structure within the four different Berea samples was studied using a combination of X-ray computed tomography, mercury injection porosimetry and high resolution scanning electron microscopy. Results show that two Berea sandstone permeability ranges have a bimodal pore-throat-size distribution whereas the other two were dominated by a unimodal pore-throat size distribution. SEM imaging of the pore network showed that permeability is mainly controlled by pore connectivity in the clay mineral matrix. Next to the pore connectivity, three-dimensional pore space showing both pore-to-pore and pore-to-pore-throat-to-pore relationships are also important.

18/00036 ν-X-type relative permeability curves for steam-water two-phase flows in fractured geothermal reservoirs

Watanabe, N. *et al. Geothermics*, 2017, 65, 269–279.

This study explored appropriate relative permeability curves for steam-water two-phase flows in fractured geothermal reservoirs through steam-water and nitrogen gas-water two-phase flow experiments and simulations on a single fracture and multiple fractures in granite under confining stress. Based on this analysis, new relative permeability curves were proposed, these consisted of ν- and X-type curves for single fractures. The ν-X-type relative permeability curves appear to reproduce Icelandic field data for steam and water relative permeabilities, which are difficult to reproduce by porous-rock-type relative permeability curves, indicating that the ν-X-type relative permeability curves are appropriate for steam-water two-phase flows in fractured geothermal reservoirs.

18/00037 Optimal control of ICV's and well operating conditions for the water-alternating-gas injection process

Chen, B. and Reynolds, A. C. *Journal of Petroleum Science and Engineering*, 2017, 149, 623–640.

Water-alternating-gas (WAG) injection is a well-known enhanced-oil-recovery (EOR) method in the oil industry. In a previously published paper, the authors concluded that the estimated net-present-value (NPV) of WAG flooding can be improved significantly by applying life-cycle production optimization. However, when reservoir layers have significantly different petro-physical properties, WAG can result in early breakthrough of the injected water and/or injected gas in layers with unfavourable physical characteristics. Thus, the production optimization technology used previously may result in a lower NPV or cumulative oil produced than can be obtained if the injection and/or production rates can be controlled on a layer-by-layer base. Recently, intelligent or smart completions, such as inflow control valves (ICVs), have been used to optimize well performance. When ICVs are installed in wells, it allows us to optimize the production/injection well controls of perforated segments along the wellbore to maximize NPV or sweep efficiency and water and/or gas breakthrough. This work considers smart completions for both injection and production wells. The authors optimize the well controls (rates or pressures) and ICV settings simultaneously and compare the NPV obtained by this process with the NPV obtained by optimizing only well controls and with the NPV generated by optimizing only ICV settings.

18/00038 Overpressure characteristics and effects on hydrocarbon distribution in the Bonan Sag, Bohai Bay Basin, China

Liu, H. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 811–821.

Overpressure is widespread in the Bonan Sag of the Bohai Bay Basin, East China, and has a strong influence on the migration and accumulation of hydrocarbons sourced from the Es3 and Es4 formations. Pressure measurements in drill stem tests and estimates from sonic logs yield overpressures among different reservoirs and mudstone beds. The fluid pressure in the Bonan Sag increases with depth and is divided into the upper, middle and lower overpressure units that correspond to the Es1, Es3 and Es4 formations, respectively. Oil–source correlation suggests that the distribution of hydrocarbons generated from Es3 and Es4 is controlled by the three pressure units. Hydrocarbons generated from Es4 source rock may laterally migrate within sandstones and accumulate in reservoirs in the Es4 Formation due to the gypsum seal in the lower overpressure unit. A small amount of hydrocarbons vertically migrated along active faults into a shallow formation during charging. However, the effects from faults were more significant on the migration and accumulation of hydrocarbons from the Es3 shale source in the middle overpressure unit. Hydrocarbons generated from the Es3 source rock can vertically migrate into the Es2 or Es1 reservoirs; however, most of them accumulated in Es3 reservoirs. Therefore, the exploration interval should be within the middle and lower overpressure units in the Bonan Sag or along the active fault within the upper overpressure unit.

18/00039 Regeneration of channelized reservoirs using history-matched facies-probability map without inverse scheme

Lee, K. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 340–350.

Reservoir characterization is a key step to define the facies connectivity in channelized reservoirs. Recently, a new paradigm combining production data with geostatistics has been proposed. Pseudo-hard and -soft data are prepared from production-based techniques, such as ensemble-based methods. However, these methods contain inverse algorithms to integrate dynamic data and have limitations in their uncertainty quantifications on new production wells. In this study, a novel approach for re-static modelling scheme is proposed by history-matched facies-probability map without inverse modelling. Initial static models are realized and selectively simulated for centre models, which are chosen by a distance-based method to reduce the number of forward simulation. The average of the selected models, which have a low level of mismatch with the observed data, is used for regeneration of facies models as facies-probability map. Regenerated channelized models are assessed again following the same procedure to select the final models. When the proposed method is applied to a 2D synthetic case, the final models successfully describe the true channel connectivities and facies ratios. Furthermore, the models preserve the bimodal distribution and given well data. Future productions for both the pre-existing production wells and a newly drilled well are properly predicted by the final models. In terms of the simulation time, the proposed method significantly decreases to 30 times from 800 times of the forward simulations over the ensemble smoother case.

18/00040 Sequential deep eutectic solvent and steam injection for enhanced heavy oil recovery and in-situ upgrading

Mohsenzadeh, A. *et al. Fuel*, 2017, 187, 417–428.

Recently, deep eutectic solvents (DESs) have been introduced and investigated as new EOR agents for heavy oil recovery enhancement. In this study, sequential DES and steam flooding was proposed and experimentally investigated as a new scenario for heavy oil recovery enhancement and having potentials for *in situ* heavy oil upgrading. DESs used in this study are choline chloride : glycerol (DES1) and choline chloride : urea (DES2). Primary and secondary DES flooding at different concentration followed by high-temperature steam flooding were conducted using 16.5 °API heavy oil and Berea sandstone core plugs. DES thermogravimetric analysis (TGA) performed and results verified the relatively high thermal stability of the selected DESs. Maximum decomposition temperature was found to be 320 and 370 °C for DES1 and DES2, respectively. This improves their potential for use as chemical additives or pre-flooding agents in thermal EOR methods. Sequential steam flooding after undiluted and two-fold diluted DES injection recovered an additional heavy oil of 12% IOIP compared to steam flooding alone. However, using more diluted solutions (i.e. 20-fold diluted DESs) caused the same and in some cases lower total recovery factor by secondary steam flooding. When followed by steam flooding, DES2 exhibited superior heavy oil recovery enhancement (8–12%) compared with DES1 (1.5–6%) at the same concentrations. Analysis of physicochemical properties of produced oil for different cases revealed the favourable role of DES in upgrading the *in situ* heavy oil. Heavy oil upgrading were quantified through various measurements including increase in API gravity up to 3.5 °API, 16.6% reduction in sulfur content or desulfurization and increase in the yields of saturate hydrocarbons. Comparatively, DES1 exhibited better overall performance than DES2 in terms of *in situ* heavy oil upgrading.

18/00041 Smectite-illitization difference of source rocks developed in saline and fresh water environments and its influence on hydrocarbon generation: a study from the Shahejie Formation, Dongying Depression, China

Li, Y. *et al. Marine and Petroleum Geology*, 2017, 80, 349–357.

Samples of argillaceous source rocks from three sub-members of the Shahejie Formation (Es) in the Dongying Depression, China, were collected to investigate the differences in hydrocarbon generation among the sub-members, which developed in fresh (Es_3^2, Es_3^3) and saline (Es_4^1) water environments. Pyrolysis, XRD and thermo-XRD analyses were used to compare the characteristics of organic matter (OM), clay minerals and OM occurrences. Total organic carbon and hydrocarbon potential proxies suggest that the samples from Es_3^3 were much better than the other two intervals, which agrees with previous studies. The characteristics of clay minerals suggest that the samples from Es_4^1 have the most abundant illite, with a maximum illite percentage in mixed-layer illite-smectite (I–Sm), and the best crystallinity of I–Sm with a main stacking mode of R1.5. However, the stacking modes of I–Sm in Es_3^2 and Es_3^3 were primarily R0 and R1, respectively, and the crystallinity was relatively poor. Thus, the smectite illitization process was faster in Es_4^1 than in the other two intervals, and a saline environment was a primary cause for the acceleration of the process. Moreover, OM occurrence indicates that the samples from Es_4^1 had the lowest amount of interlayer OM, whereas Es_3^3 had the largest amount. Therefore, the rapid illitization in Es_4^1 caused abundant interlayer OM to be desorbed and discharged, which in turn caused the amount of residual interlayer OM in Es_4^1 to be less than that in the other two intervals. Thus, the source rocks of Es_4^1 made a more significant contribution to hydrocarbon generation than those of the other two units. In conclusion, the inconsistent illitization among these intervals was a major cause of the differences in hydrocarbon generation.

18/00042 The Messinian event in the Paratethys: astronomical tuning of the Black Sea Pontian

Rostovtseva, Y. V. and Rybkina, A. I. *Marine and Petroleum Geology*, 2017, 80, 321–332.

This study presents new data on the orbitally calibrated Maeotian/Pontian and Pontian record of the Black Sea Basin (Paratethys) obtained by time-series analysis of magnetic susceptibility (MS) data from relatively deep-water Upper Miocene sediments exposed in the Zheleznyi Rog section (Taman Peninsula, Russia). In the studied interval, a ~145-m-long sedimentary sequence, spectral analysis revealed statistically significant signals with 6.1–8.2 m and 3.0–4.0 m wavelength. These signals correspond to the obliquity and precession cycles, respectively. This study correlates the main steps of Messinian salinity crisis (MSC) of the Mediterranean to the Black Sea Pontian record based on astronomical tuning of the study sequence and evaluation of integrated biostratigraphic, paleomagnetic and sedimentological data. Based on cyclostratigraphic results, Maeotian/Pontian beds with *Actinocyclus octonarius* accumulated from ~6.3 to 6.1 Ma. Most of the Novorossian sediments correspond to the first MSC step. The TG 22 (5.79 Ma) and TG 20 (5.75 Ma) glacial events occur in the uppermost Novorossian record and are marked by extraordinary high values of MS. The Portaferian, dated at the base as ~5.65 Ma and the top as ~5.45 Ma, corresponds to the second MSC step. The Novorossian/Portaferian transition is marked by the hiatus of approximately 150–160 kyr, which agrees well with the concept of the intra-Pontian unconformity in the Black Sea Basin and a sea-level drop in the Mediterranean from 5.6 to 5.46 Ma. The ages for the base and the top of the Bosphorian were estimated as ~5.45 Ma and ~5.27 Ma, respectively. The base of the Bosphorian corresponds to the third Lago Mare episode caused by the high sea-level connection between the Mediterranean and Eastern Paratethys.

18/00043 The role of metalloporphyrins on the physical-chemical properties of petroleum fluids

Silva, H. S. *et al. Fuel*, 2017, 188, 374–381.

The presence of metalloporphyrins in crude oil has been known by many years now but their role on the physical-chemical properties of petroleum fluids, such as the aggregation of the high-molecular weight phases, remains unknown. In this paper, these properties are studied using different molecular modelling techniques (molecular dynamics, semi-empirical PM7 and density functional theory). This combined methodology allowed us characterizing the nature of these interactions, how it dominates the electronic structure of the stacked molecules and what is their participation on the formation of the nano-, micro- and macro-aggregates.

18/00044 Towards the understanding of microbial metabolism in relation to microbial enhanced oil recovery

Halim, A. Y. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 151–160.

In this study, *Bacillus licheniformis* 421 was used as a model organism to understand the effects of microbial cell growth and metabolite production under anaerobic conditions in relation to microbial enhanced oil recovery. The bacterium was able to grow anaerobically on different carbon compounds, where n-alkanes were preferred over molasses as carbon source. The bacterium grew slowly when n-alkanes were used as carbon source, however, formation of emulsion and reduction of interfacial tension (IFT) were still observed. The bacterial cells were mainly present at the interface of the synthetic seawater medium and the n-alkanes. The bacterium produced lipopeptide lichenysin G which was detected both in the water and in the emulsion phase. It is proposed that the bacterial cells themselves or metabolites attached to the cell surface are the main players in the formation of emulsions and IFT reduction.

18/00045 Vanadium, nickel and sulfur in crude oils and source rocks and their relationship with biomarkers: implications for the origin of crude oils in Venezuelan basins

López, L. and Lo Mónaco, S. *Organic Geochemistry*, 2017, 104, 53–68.

This work presents a study of vanadium, nickel and sulfur concentrations and biomarkers in a suite of crude oils and source rocks from three Venezuelan basins (Maracaibo and Eastern basins and Barinas sub-basin). Crude oils range from unaltered to altered by biodegradation, and source rocks are characterized by having different kerogen types (Type II, III or IV) and maturity levels (early mature to post-mature). Vanadium, nickel and sulfur concentrations, V/Ni or V/(V + Ni) and saturate biomarkers were used to classify the oils and source rocks based on inferred paleo-redox environment, lithology and maturity of the source rock. Oils are classified into five groups based on V/Ni ratios; they appear to be related to variations in the paleo-redox environment (from suboxic-dysoxic to anoxic-suboxic) of source rocks with variable lithological composition and organic matter input, regardless of their maturity or biodegradation level. These five groups are also classified based on biomarkers related to maturity, organic matter type, paleo-redox environment and source rock lithology. In source rocks, vanadium, nickel and sulfur concentrations, together with V/Ni or V/(V + Ni) ratios, provide information about the paleo-redox environment and are related to lithology, regardless of their maturity. These results also indicate variable paleo-redox conditions during the sedimentation of Venezuelan source rocks. All this suggests that, while the main source rocks in Venezuelan basins are well established, there are still uncertainties regarding their lateral and vertical variations in organic and inorganic facies and paleo-redox conditions. The presence of other source rocks contributing to the accumulation of hydrocarbons in the Venezuela basins is also a possibility.

18/00046 Wave-induced seabed response around an offshore pile foundation platform

Zhang, Q. *et al. Ocean Engineering*, 2017, 130, 567–582.

In this paper, a three-dimensional integrated numerical model including the wave and seabed sub-model is developed to investigate the wave induce seabed response around a pile foundation platform. The wave sub-model is based on volume-averaged Reynolds-averaged Naiver–Stokes (VARANS) equations with k-ε turbulence closure scheme, and the volume of fluid (VOF) method is applied to track water free surface. The seabed is treated as an isotropic and homogeneous porous medium and characterized by Biot's partly dynamic equations (u–p model). The proposed model is verified with the previous analytical results. Based on the numerical results, the distribution of flow field around pile foundation will be investigated. Then, a comprehensive comparison between a pile foundation platform model and a pile foundation without platform model will be performed to examine the effects of platform to the pile foundation. Finally, the effects of wave, pile foundation, and seabed characteristics, such as wave depth, wave height, pile diameter, pile insertion ratio, soil permeability and degree of saturation on the wave-induced seabed and pile foundation platform response will be studied.

Transport, refining, quality, storage

18/00047 A parabolic solvent chamber model for simulating the solvent vapor extraction (VAPEX) heavy oil recovery process

Ma, H. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 465–475.

During the solvent vapour extraction (VAPEX) process, a heavy oil reservoir can be divided into three different zones in terms of its fluid saturations, namely, the solvent chamber, transition zone, and untouched heavy oil zone. In the past, the solvent chamber was assumed to be a linear or circular shape in the previous studies. However, it has been observed to be close to a parabolic shape in many laboratory VAPEX tests. In this paper, a new parabolic solvent chamber model in the concave or convex case is formulated to predict the solvent chamber evolution and the heavy oil production in the VAPEX heavy oil recovery process. In the experiment, each recorded digital solvent chamber image at a different time is digitized to determine the solvent chamber shape by analysing the sudden change of the gray level of each pixel. In theory, the overall discrepancy between the predicted and

digitized solvent chambers is minimized by adjusting the transition-zone thickness. It is found that in comparison with the linear and circular solvent chamber models, the parabolic solvent chamber model gives the best prediction of the solvent chamber evolution, especially in the spreading phase. In addition, the maximum transition-zone thickness variation of 13.1% during the entire VAPEX test indicates that the transition-zone thickness can be assumed to be constant. Similar to the other solvent chamber models, the parabolic solvent chamber model can adequately predict the cumulative heavy oil production. The relatively large error of the predicted cumulative heavy oil production is caused by a commonly used assumption. The initial oil saturation in the transition zone is assumed to reduce to the residual oil saturation once the transition zone becomes an incremental part of the solvent chamber. This major theoretical assumption needs to be further investigated.

18/00048 Development of anionic-cationic inhibitors for mitigating silicate scales during ASP flooding

Mahat, S. Q. A. and Mohd. Saaid, I. *Journal of Petroleum Science and Engineering*, 2017, 149, 701–706.

Silicate scaling is often induced by alkaline surfactant polymer (ASP) flooding in sandstone reservoirs. The formation of silicate scale is complicated by its dependence on multiple factors including pH, silica concentration, and magnesium concentration, which vary as the flood progresses. These factors affect silicate scaling tendency, and consequently, severity of the problem. Silicate scale is a very serious problem in the oil and gas production system. Therefore, silicate scale inhibitors have been suggested to mitigate problems in oilfields. In this study, some of the dendrimers inhibitors with enhanced functionality used in the water industry were reviewed and assessed for possible application in oilfields scales. It was found that the NH_2-terminated dendrimers exhibited excellent inhibitory silica polymerization efficiency compared with the control. It is now certain that effective silica scale inhibition is dependent on the cationic charge on the polymer backbone. However, these dendrimer inhibitors suffered from a serious disadvantage when the silicates that had not been inhibited entrapped the dendrimers. Visual observations showed that these particles appeared as white flocculant precipitates at the bottom of the test vessels. Previously, it had been found that silica scale inhibition could be achieved by using of scale inhibitors in combination with anionic polymer additives. It is believed that an effective silica inhibition should be based on a delicate balance structure of cationic–anionic charges. Therefore, in the present study pteroyl-L-glutamic acid (PGLU) compound is used in synergistic action with cationic dendrimer polymer. PGLU was proven to be an effective scale inhibitor at high temperature in aqueous solution of synthetic produced water. Furthermore, it was found that PGLU assisted the inhibitory action of dendrimers by alleviating formation of insoluble SiO_2-PAMAM precipitates to operate more effectively.

18/00049 Effects of oil cracking on fluorescence color, homogenization temperature and trapping pressure reconstruction of oil inclusions from deeply buried reservoirs in the northern Dongying Depression, Bohai Bay Basin, China

Ping, H. *et al. Marine and Petroleum Geology*, 2017, 80, 538–562.

The effects of oil cracking on fluorescence colour, homogenization temperature (T_{ho}) and trapping pressure (P_t) of oil inclusions from deeply buried reservoirs (DBRs) (3672–4359 m) in the northern Dongying Depression were determined based on fluorescence spectroscopy and homogenization temperatures of oil inclusions, kinetic modelling of crude oil cracking, and petroleum inclusion thermodynamics modelling. The modelling results demonstrate that fluorescence colour, T_{ho} and predicted P_t have strong relationships with the transformation rate via cracking of oil to gas (T_r), and the formation temperature (T_f) that the inclusions experienced. The fluorescence colour is hardly influenced at all during the initial stages of oil cracking ($T_r < 13\%$, $T_f < 160\,°C$), but fluorescence color begins to shift toward shorter wavelengths (blue shift) during progressive oil cracking ($T_r < 24\%$, $T_f < 190\,°C$). With further oil cracking, the fluorescence colour may either experience no change or continue its blue shift. Eventually the fluorescence colour will disappear as the aromatic compounds are completely cracked. The T_{ho} increases at first ($T_r < 24\%$, $T_f < 190\,°C$), but then decreases or even becomes negative during major oil cracking. The reconstructed P_t values show a corresponding reverse trend. Oil inclusions from DBRs and other shallow reservoirs in the Dongying Depression show an obvious blue shift in fluorescence colour at a depth of approximate 4000 m ($T_f = 160\,°C$) and generally contain solid bitumen below 4000 m, supporting the effect of oil cracking on fluorescence variation, consistent with the modelling result. The T_{ho} from DBRs in the Minfeng area increases with increasing burial depth ($T_f < 190\,°C$), which is also consistent with the modelling results. However, the T_{ho} of oil inclusions with blue-white fluorescence from DBRs in the Shengtuo area did not show such a trend. Recent trapping, high trapping pressure and higher-maturity oil may have led to a low-degree of oil cracking, and thus less modification of T_{ho} in the Shengtuo area. Oil cracking results in consistent volume ratios of pyrobitumen to oil inclusions (F_{vpy}) in the same fluid inclusion assemblage, and the F_{vpy} value increases with oil cracking level, which can be used to recognize if oil cracking has occurred in oil inclusions and what level of oil cracking they have experienced. As the oil cracking model used in this study did not account for the role of pressure, it is more applicable for oil inclusions that were trapped under normally pressured conditions. Oil inclusions trapped under overpressured conditions will be less influenced by oil cracking.

18/00050 Experimental study on pressure control strategies for improving waterflooding potentials in a heavy oil-methane system

Peng, X. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 126–137.

Due to the adverse mobility ratio conditions in heavy oil waterflooding processes, the viscous force is not as significant as that in conventional waterflooding in terms of enhancing oil recovery. Instead, pressure related mechanisms, such as foamy oil flow and solution gas drive, might have significant effects on waterflooding performances when an operating strategy is beneficial (e.g. voidage replacement ratio less than one). In this study, a series of waterflooding tests are performed to study the beneficial operating strategies in a heavy oil-methane system from the pressure control aspect. The pressure control strategies include primary-ended waterflooding (Strategy 1), primary-plus waterflooding (Strategy 2), pseudo-continuous injection with cyclic production (Strategy 3) and cyclic injection with cyclic production (Strategy 4). The depletion rates include 0.45, 1, 2 and 3 kPa/min. Experimental results show that the optimal pressure control strategy for the heavy oil–methane system is Strategy 2. The ultimate oil recovery and overall average production rate are inversely changed with the depletion rate increasing in Strategy 2. To get a balance between the ultimate oil recovery and overall average production rate, the optimal depletion rate, 2 kPa/min, is obtained. By comparing the performances of Strategy 2 under different depletion rates, the relationship of voidage displacement ratio (VRR) with the depletion rate as well as the optimal VRR for waterflooding are obtained. Moreover, it is found that, with depletion rate increasing, positive effects of depletion rate decrease at foamy oil flow stage and increase at solution gas drive stage.

18/00051 Extraction of crude oil from petrochemical sludge: characterization of products using thermogravimetric analysis

Hu, J. *et al. Fuel*, 2017, 188, 166–172.

In this study, solvent extraction was used to recover oil from petrochemical sludge. Three solvents were chosen to mix with petrochemical sludge to ensure adequate miscibility of crude oil in solvent under an appropriate condition. The petrochemical sludge, crude oil sample and residual petrochemical sludge were analysed by thermogravimetric analysis (TGA). The experiments were performed at three different heating rates (10, 20, 30 °C/min) under nitrogen atmosphere. The aim of the study was to recover and evaluate crude oil from petrochemical sludge and assess the commercial potential of recycling the crude oil. Experimental results showed that the common temperature range of weight loss of the crude oil sample was about 200–550 °C. The residual petrochemical sludge still remained the partial characteristics of petrochemical sludge, which demonstrated that the residual petrochemical sludge still had the value of exploiting and utilizing for further research.

18/00052 Incidence of load combination methods on time-variant oil tanker reliability in intact conditions

Campanile, A. *et al. Ocean Engineering*, 2017, 130, 371–384.

Reliability analysis of an oil tanker in intact conditions is performed to investigate the incidence of load combination methods on hull girder sagging/hogging time-variant failure probability. Particularly, Turkstra rule, Ferry Borges and Castanheta method and Poisson square wave model are applied to evaluate the statistical distribution of bending moment, with reference to both one voyage and 1-year period. Statistical properties of time-variant ultimate strength are determined by Monte Carlo simulation, up to 25-year ship lifetime; bending capacity is determined by means of a modified incremental-iterative method, to account for corrosion wastage of structural members contributing to hull girder strength, welding residual stresses and material properties randomness. After determining the still water load combination factors, based on statistical properties of still water, wave and total vertical bending moments, with reference to 1-year time interval, reliability analysis is performed by Monte Carlo simulation, based on limit state formulations relative to different load combination methods. Finally, the VLCC double hull oil tanker, benchmarked in the 2012 ISSC report, is assumed as a reference ship and obtained results are fully discussed.

Economics, business, marketing, policy

18/00053 Molecular composition assessment of biodegradation influence at extreme levels – a case study from oilsand bitumen in the Junggar Basin, NW China

Huang, H. and Li, J. *Organic Geochemistry*, 2017, 103, 31–42.

In order to understand the effects of extreme biodegradation on petroleum molecular compositions, a series of shallow buried oil sands from the north-western margin of the Junggar Basin, north-west China has been investigated using geochemical methods. Most samples have experienced at least level 8 biodegradation on the scale of Peters and Moldowan, but their molecular compositions still show dramatic variations. The bi- and tricyclic aromatic compounds are almost completely removed with aromatic steroid hydrocarbons being the only visible molecules in the aromatic hydrocarbon fraction. However, aromatic steroids are not sensitive to the assessment of biodegradation extent possibly due to mixed effects with water washing. At an extreme level of biodegradation after diasteranes were attacked, pregnanes, tri- and tetracyclic terpanes, non-hopane pentacyclic terpanes such as 18α-30-norneohopane, C_{30} diahopane and gammacerane remain prominent. The post extreme level of biodegradation can be further differentiated on the basis of the presence and absence of these 'refractory' components together with 25-norhopanes (NHs), 17-nortricyclic terpanes (NTTs) and C_{23} demethylated tetracyclic terpane (C_{23}NTeT). These NHs, NTTs and C_{23}NTeT are produced from corresponding hopanes, tri- and tetracyclic terpanes during biodegradation but they are biodegradable as well. Extreme plus 1 level of biodegradation is characterized by the attack of pregnanes and tricyclic terpanes. Extreme plus 2 level of biodegradation is characterized by the attack of tetracyclic terpanes and non-hopane pentacyclic terpanes. When biodegradation level reaches to extreme plus 3, NHs and NTTs are largely depleted. At extreme plus 4 level, the only traceable components are C_{23}NTeT and C_{29}NH. While different basins or reservoirs may have their unique features of the biodegradation process, relative rates of biodegradation of the different hydrocarbon classes that occur in the Junggar Basin may provide a protocol for intensity assessment after the extreme level of biodegradation is reached.

18/00054 Solvent demetallization of heavy petroleum feedstock using supercritical carbon dioxide with modifiers

Magomedov, R. N. *et al. The Journal of Supercritical Fluids*, 2017, 119, 150–158.

Possibilities of demetallization of heavy petroleum feedstocks (HPF) using supercritical fluid extraction (SFE) have been studied. Experiments with various solvent mixtures were carried out in a semibatch extractor and in dynamic mode to assess the effect of modifier type and concentration as well as extraction time on the yield of extract and content of vanadium, nickel and iron in produced phases (extract and residual phase). Vacuum residue was used as the feedstock and supercritical carbon dioxide ($scCO_2$) was used as the primary solvent for extraction. Methanol, ethanol, acetonitrile, acetone, ethyl acetate, *n*-heptane, toluene and o-xylene were added to $scCO_2$ as modifiers to form the solvent mixtures. Extraction temperatures and pressures were maintained at 50 °C and 30 MPa to achieve a high density of $scCO_2$. It has been found that methanol and o-xylene containing mixtures provide the highest metal content in the extract while ethyl acetate, *n*-heptane and toluene provide the lowest. Higher extract yield and the degree of metal concentration in residue were obtained with increasing both toluene concentration in $scCO_2$ and the time of dynamic extraction. The demetallization efficiency is estimated to be at a level above 95wt % at the yields of extract (demetallized oil) up to 60wt % using toluene as a modifier.

18/00055 Total resistance prediction of an intact and damaged tanker with flooded tanks in calm water

Bašiá, J. *et al. Ocean Engineering*, 2017, 130, 83–91.

This paper presents the prediction of the total resistance of an intact and damaged ship model using the computational fluid dynamics (CFD) technique. The study is performed on the model of a tanker with a large hole in the bottom of the hull. The damage is based on statistical data on ship grounding accidents and the chosen hole size and location in the midship area represents its plausible size and location due to grounding. Reynolds-averaged Navier–Stokes equations with the volume of fluid surface capturing technique are employed to solve the flow around the steadily advancing model of a damaged ship in calm water. The experiments, both on an intact and a damaged ship model that were carried out in the towing tank of the Brodarski Institute in Zagreb, Croatia, are used to evaluate the results. The numerical results are in a good agreement with the experimentally obtained results. The significant average increase of 27% in total resistance due to the altered flow around the hole and inside the flooded tanks can be observed for the analysed case. The study shows that the proposed CFD model and settings provide a good prediction of the total resistance together with the flow both around the damaged hull and inside the flooded tanks of the damaged tanker.

18/00056 An improved deconvolution algorithm using B-splines for well-test data analysis in petroleum engineering

Liu, W. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 306–314.

Ilk *et al.*'s deconvolution algorithm using B-splines involves the Laplace transformation of the convolution equation with respect to production rate and wellbore pressure based on Duhamel principle. However, for common cases, the production rate function has 'discontinuity' with respect to production time; it does not satisfy the precondition that the function to be transformed by Laplace transformation should be continuous. This inherent defect may directly cause enormous amount of computational time or even the failure of the numerical Laplace inversion in the deconvolution process. Based on these concerns, a fundamentally improved deconvolution algorithm using B-splines is presented here. In the convolution equation, the wellbore pressure derivative corresponding to constant unit production rate as the target of deconvolution is still represented by weighted summation of second-order B-splines; however, the computation process of the deconvolution is kept in the level of integral in the real time space instead of the Laplace space, for the reason that there will be no continuity requirement for the production rate function in the application of Duhamel principle for the deconvolution computation problem. According to the real production rate history, a technique of piecewise analytical integration is adopted for obtaining the elements of sensitivity matrix of a linear system with respect to weight coefficients; the linear system is generated by substituting the measured wellbore pressure data and corresponding variable production rate data into the convolution equation containing B-splines. The proposed direct analytical solution method of the integration for calculating the elements of the sensitivity matrix can not only guarantee the success of the deconvolution computation, but also can largely enhance the deconvolution computation speed. Moreover, in order to further improve the computation speed, a binary search method is also applied to find which production segments (with constant production rate) the measured wellbore pressure data points locate at in the deconvolution computation process. Another linear system with respect to weight coefficients for the regularization from Ilk *et al.*'s deconvolution algorithm is appended in order to overcome the effect of data errors. The two linear systems are combined together as an over-determined linear system, which can be solved by the least square method. Eventually, the reconstructed wellbore pressure and its derivative by B-splines corresponding to the constant unit production rate can be obtained. Numerical experimental tests demonstrate that the improved deconvolution algorithm exhibits good accuracy, computation speed and stability of data error tolerance. And the statement on how to perform the regularization when data error exists is also made in order to deconvolve the correct wellbore pressure derivative. The improved deconvolution algorithm is also applied into an actual field example. It is found that the deconvolution results by the improved deconvolution algorithm have good agreement with the ones by von Schroeter *et al.*'s deconvolution algorithm and by Levitan *et al.*'s deconvolution algorithm as a whole; and the feature of typical log-log curves of the wellbore pressure drop and the wellbore pressure derivative corresponding to the improved algorithm is very close to the one of typical log-log curves calculated directly from the wellbore pressure data in the well shut-in period. In addition, through many numerical experimental tests, it is also concluded that as the quantity of data largely increases, the improved Ilk *et al.*'s deconvolution algorithm exhibits the big advantage in fast computational speed over von Schroeter *et al.*'s algorithm and Levitan *et al.*'s algorithm.

18/00057 Another look on the relationships between oil prices and energy prices

Lahiani, A. *et al. Energy Policy*, 2017, 102, 318–331.

This paper employs the quantile autoregressive distributed lags (QARDL) model to investigate the pass-through of oil prices to a set of energy prices. This approach allows analysing simultaneously short-term connections and long-run cointegrating relationships across a range of quantiles. It also provides insights on the short-run predictive power of oil prices in predicting energy prices while accounting for the cointegration between oil prices and each of the considered energy prices in low, medium and high quantiles. Two key findings emerge from this paper. First, all considered energy prices are shown to be cointegrated with oil price across quantiles meaning that a stationary equilibrium relationship exists between single energy price and oil price. Second, the authors find evidence that oil price is a significant predictor of individual petroleum products prices and natural gas in the short run. This paper has important policy implications for forecasters, energy policy-makers and portfolio managers.

18/00058 Crude oil price behaviour before and after military conflicts and geopolitical events

Monge, M. *et al. Energy*, 2017, 120, 79–91.

Crude oil price behaviour depends on all the events that have the potential to disrupt the flow of oil. These causes could be due to geopolitical issues and/or military conflicts in/with the producer countries and a problem relating to demand and supply. This paper first investigates the statistical properties of the real oil prices as well as its log-transformation, along with the absolute and squared returns values. Then, the authors address the following issue: does the crude oil price behave in the same way before and after a military conflict or geopolitical problem in the producer countries? To answer this question the real oil prices of West Texas Intermediate (WTI) were analysed before and after the different military conflicts and political events that occurred after the Second World War. For this purpose techniques were used based on unit roots and fractional integration. The empirical results provide evidence of persistence and breaks in the oil prices series and stationary long memory in the absolute returns. However, significant differences were observed before and after the conflict and geopolitical events.

18/00059 Evaluation of feasibility index in the arrangement design of an offshore topside based on the automatic transformation of experts' knowledge and the fuzzy logic

Kim, S.-K. *et al. Ocean Engineering*, 2017, 130, 284–299.

In an offshore platform, many modules and equipment are placed on the limited space called topside, so that the space should be used efficiently. Furthermore, a sufficient space between equipment should be provided for the operability, maintainability, and safety. To guarantee suitable arrangement design, there are many requirements to be considered such as international codes and standards, including owners' own requirements. Meanwhile, the arrangement design of an offshore topside tends to rely on experts' knowledge and experiences. Due to the heavy dependence on experts' knowledge and experiences, consequently, a different arrangement can be derived according to a personal disposition, in spite of the same requirements. In addition, an unacceptable arrangement can be derived due to the omission of some requirements by a designer. To solve such problems, an expert system for the arrangement design of an offshore topside was proposed based on an arrangement evaluation model (AEM) in this study by expanding the previous study of authors for the arrangement design of a submarine. In addition, an arrangement template model (ATM) was proposed to store various data on the arrangement design of the offshore topside. To evaluate the applicability of the proposed expert system, a prototype program consisting of the AEM and the ATM was also developed here. Finally, this programme was applied to a problem of a large FPSO topside. The results showed that the proposed system can be used to evaluate the given alternatives for the arrangement design of the offshore topside.

18/00060 Falling oil prices: causes, consequences and policy implications

Khan, M. I. *Journal of Petroleum Science and Engineering*, 2017, 149, 409–427.

Following 4 years of high stable prices at about $107 per barrel, crude oil prices have fallen sharply since summer 2014 and are projected to stay at low level for an extended period. While there are multiple factors under consideration, most observers have conjectured that the domestic oil boom in the USA and Iraq is the major cause for the falling oil prices. Some have suggested that a major shock to oil price expectations occurred after the November 2014 meeting of OPEC, when they did not cut production despite the steady increase in non-OPEC oil production. In the first part of the publication, the authors quantitatively analysed the effect of various factors on the oil prices and then studied the contribution of the geopolitical strategies of the USA and Saudi Arabia towards this oil crash. They conducted a comparative analysis of the recent drop in oil prices with previous incidents up to 1996. This showed that the demand and supply formula cannot be implemented in the face of the current plunge in oil prices. The authors studied the economic and financial consequences of the falling oil price and finally they discuss the projections of oil prices.

18/00061 Investigating diesel market integration in France: evidence from micro data

Cárdenas, J. *et al. Energy Economics*, 2017, 63, 314–321.

This study uses station-level daily price observations collected over a period of eight years to study the extent of diesel market integration in France. The empirical analysis starts off by examining the time-series properties of diesel price ratios, and then assesses how geographical separation and petrol station characteristics affect the speed of adjustment of prices to exogenous shocks. The findings reveal that the great majority of diesel price ratios maintain stable long run relationships. It was also found that while price ratios take longer to adjust for pairs of petrol stations that are farther apart, adjustment is quicker when pairs of petrol stations provide the same range of services, and when they belong to the same owner.

18/00062 Measuring the benefit of investing in pipeline safety using fuzzy risk assessment

Urbina, A. G. and Aoyama, A. *Journal of Loss Prevention in the Process Industries*, 2017, 45, 116–132.

This study introduces a framework to evaluate the benefits of investing in safety measures for pipelines using fuzzy logic as a tool to deal with uncertainty. Using the possibility theory of fuzzy logic, this paper provides a way to determine the surplus between the amount of risk mitigated and the costs of the activities associated with such mitigation. The framework thereby allows pipeline operators to determine whether the costs associated with these risk management activities are reasonable or not despite the common degree of uncertainty of the data derived from the lack of information or subjective judgment. The proposed model considers variables such as threat and consequence scenarios, probability of adverse events, vulnerability, failure modes, percentages of risk reduction and mitigation costs. Furthermore, this framework is developed using the fuzzy inference system toolbox of MATLAB, employing specifically the Mamdani algorithm with a triangular membership function. To illustrate the relevance of the assessment of the value-added by safety management, this paper presents an application case from the oil and gas network of Colombia. The results of this case show that although the general trend of the net value for the safety activities is positive, there are some areas in which the investment in safety is significantly less cost effective. The data indicates that for a length corresponding to the 29% of the pipeline, the costs of the safety measures are bigger than the risk mitigated. Also, the results show that it is possible to estimate an investment ratio for safety measures, which for the application case is 5.41% with a net benefit of $50 million in risk reduction.

18/00063 On the rate of return and risk factors to international oil companies in Iran's buy-back service contracts

Ghandi, A. and Lawell, C.-Y. C. L. *Energy Policy*, 2017, 103, 16–29.

This study analysed the rate of return (ROR) and risk factors faced by Shell Exploration, an international oil company (IOC), in its Soroosh and Nowrooz buy-back service contract in Iran. In particular, based on models of cash flow, the authors analyse the buy-back contract specific risk factors that can contribute to a reduction in the rate of return for the international oil company. The cash flow models resemble the cash flow of buy-back service contracts before the Iranian government changed the way it determined the capital cost ceiling and pre-defined the oil price in these contracts in 2008–2009. The actual and contractual cash flow models reveal that Shell Exploration's actual ROR was much lower than the contractual level. Furthermore, it was found that among the risk factors considered, a capital cost overrun has the greatest negative effect on the IOC's ROR. Moreover, it was shown that there is a potential for modifying the contracts in order for the IOC to face an actual ROR closer to the contractual ROR even if the contract faces cost overrun or delay, without exceeding the maximum contractual ROR that the National Iranian Oil Company is willing to give.

18/00064 OPEC vs US shale: analyzing the shift to a market-share strategy

Behar, A. and Ritz, R. A. *Energy Economics*, 2017, 63, 185–198.

In November 2014, OPEC announced a new strategy geared towards improving its market share. Oil-market analysts interpreted this as an attempt to squeeze higher-cost producers, notably US shale oil, out of the market. Over the next year, crude oil prices crashed, with large repercussions for the global economy. This study presents a simple equilibrium model that explains the fundamental market factors that can rationalize such a 'regime switch' by OPEC: (i) the growth of US shale oil production; (ii) the slowdown of global oil demand; (iii) reduced cohesiveness of the OPEC cartel; and (iv) production ramp-ups in other non-OPEC countries; while (v) reductions in US shale costs act against these factors. It is shown that these qualitative predictions are broadly consistent with oil market developments during 2014–2015. The model is calibrated to oil market data; it predicts accommodation up to 2014 and a market-share strategy thereafter, and explains large oil-price swings as well as realistically high levels of OPEC output.

18/00065 OPEC's kinked demand curve

Vatter, M. H. *Energy Economics*, 2017, 63, 272–287.

Asymmetric effects of oil prices on the macroeconomy imply multiple equilibrium prices for OPEC. Here, the author estimates world demand for crude oil, non-OPEC supply, and the effects of changes in price on world GDP using quarterly data covering 1973 to 2010. If OPEC's marginal cost is $20/bbl in 2014 : III, and its discount rate is zero, estimated equilibrium prices are $44–88/bbl. Multiple equilibria

incent OPEC to tolerate unstable prices, which, because of the asymmetry, lower world GDP. Both policies that increase responsiveness to price and policies that lower net demand to OPEC narrow and lower the range of equilibrium prices, but the former are more effective at doing so. OPEC responds to changes in the discount rate in the opposite way from competitive producers, so policies that secure oil-related property rights in OPEC countries and other policies that lower OPEC's discount rate narrow and lower the range of equilibrium prices. Monetary policy is more effective at accelerating or slowing macroeconomic activity the larger is OPEC's market share.

18/00066 Potential solar energy use in the global petroleum sector
Wang, J. *et al. Energy*, 2017, 118, 884–892.
This study examines the potential for solar energy in global oil operations, including both extraction and transport ('upstream') and refining ('downstream'). Two open-source oil-sector GHG models are applied to a set of 83 representative global oil fields and 75 refinery crude oil streams (representing ~25% of global production). Results from these models are used to estimate per-barrel energy intensities (power, heat), which are scaled to generate country-level demand for heat and power. Multiple solar resource quality cut-off criteria are used to determine which regions may profitably use solar. Potential solar thermal capacity ranges from 19 to 44 GW_{th} in upstream operations, and from 21 to 95 GW_{th} in downstream operations. Potential PV deployment ranges from 6 to 11 GW_e in upstream operations and 17–91 GW_e in downstream operations. The ranges above are due to both per-bbl variation in energy intensity, as well as uncertainty in solar resource quality criteria. Potential solar deployment in upstream operations would displace a much smaller fraction of upstream energy use because a large fraction of global upstream energy use is are either offshore or in high latitude regions (e.g. Russia, Canada, central Asia).

18/00067 Pre-drill pore pressure modelling and post-well analysis using seismic interval velocity and seismic frequency-based methodologies: a deepwater well case study from Mississippi Canyon, Gulf of Mexico
Mannon, T. P. and Young, R. A. *Marine and Petroleum Geology*, 2017, 79, 176–187.
Managing and identifying risk and uncertainly involved in drilling operations in unconventional geologic settings starts with improving and correctly applying pore pressure modelling. A relatively new approach, which predicts pore pressure by way of seismic frequencies, has addressed some of the short-comings seen in seismic interval velocity applications. With the overall goal of reducing operational drilling risk by utilizing multiple pore pressure modelling strategies, a case study will be presented for a near-salt field in deepwater Gulf of Mexico. This study will outline the pre-drill pore pressure modelling, which includes petrophysical, seismic interval velocity, and seismic frequency based approaches. The accuracy of these three approaches will be analysed both qualitatively and quantitatively for currently existing wells, and from a pre-drill and post-drill standpoint for one prospect well.

18/00068 Risk analysis of using sweet sorghum for ethanol production in southeastern Brazil
Rezende, M. L. and Richardson, J. W. *Biomass and Bioenergy*, 2017, 97, 100–107.
The authors' objective was to evaluate the economic feasibility and the risks associated with the utilization of sweet sorghum as a raw material for the production of ethanol at a representative sugar mill in São Paulo State, Brazil. The economic payback of the working mill is compared with and without sweet sorghum. A sensitivity analysis of sweet sorghum yield is made to empirically estimate the risk associated with adding sweet sorghum in an ethanol mill during the sugarcane off season. The results of a Monte Carlo simulation analysis indicate that the addition of sweet sorghum on 20% of the sugarcane land can increase net present value and average annual net cash income and reduce the relative risk for net income and net present value. Given current yields for sweet sorghum in the study area, risk averse decision makers would have a risk premium benefit of about R$4.5 million per year in average annual net cash income. The analysis suggests that adding sweet sorghum to the crop mix will reduce the costs for a mill by spreading fixed costs across more ethanol. Also, an addition of sweet sorghum would increase ethanol receipts more than the variable costs of cultivating and harvesting the crop plus the costs of producing ethanol. Despite the profitability and risk reducing benefits of sweet sorghum, wide spread adoption has not occurred in south-eastern Brazil. The uncertainty about yields and effects on labour scheduling may be factors in the slow rate of adoption. Improvements in sweet sorghum yields would likely increase the rate of adoption.

18/00069 The economic viability of gas-to-liquids technology and the crude oil–natural gas price relationship
Ramberg, D. J. *et al. Energy Economics*, 2017, 63, 13–21.
This paper explores the viability of a gas-to-liquids (GTL) technology and examines how GTL penetration could shape the evolution of the crude oil–natural gas price ratio. Much research has established the cointegrated relationship between crude oil and natural gas prices in the USA. The persistently low US natural gas prices in recent years seem to mark a shift in this relationship, and have led some in industry to begin considering investments in GTL capacity in the USA. In order to look forward over decades when the underlying economic drivers may be outside of historical experience, a computable general equilibrium model of the global economy was used to evaluate the economic viability of GTL and its impact on the evolution of the crude oil–natural gas price ratio. The results are negative for the potential role of GTL. In order to produce any meaningful penetration of GTL, it was necessary to evaluate scenarios that seem extreme. With any carbon cap GTL is not viable. Moreover, even without a carbon cap of any kind, extremely optimistic assumptions about (i) the cost and efficiency of GTL technology and about (ii) the available resource base of natural gas and the cost of extraction, before the technology penetrates and it impacts the evolution of the crude oil–natural gas price ratio.

Derived liquid fuels

18/00070 A comparative thermodynamic study on the CO_2 conversion in the synthesis of methanol and of DME
Ateka, A. *et al. Energy*, 2017, 120, 796–804.
A thermodynamic approach of the synthesis processes of methanol and of DME from $H_2 + CO + CO_2$ has been conducted, in order to compare the feasibility of incorporating CO_2 in the feed of both processes. The effects of reaction temperature (200–400 °C), pressure (10–100 bar) and $CO_2/(CO + CO_2)$ ratio in the feed on the CO_2 conversion, yield and selectivity of oxygenates (methanol + DME), and heat released in each process have been studied. CO_2 conversion is strongly dependent on the CO_2 content in the feed and is higher in the DME synthesis for high CO_2 concentration values in the feed ($CO_2/(CO + CO_2) > 0.75$). The increase of reaction temperature and the increase of the CO_2 content in the feed have an unfavourable effect on the oxygenate yield and selectivity, while the increase of reaction pressure has a favourable effect. Comparing both processes, higher oxygenate yield and selectivity values are obtained in the synthesis of DME, which is more relevant for CO_2 rich feeds. Moreover, feeding CO_2 lessens the exothermic nature of both processes which is a positive effect for protecting the metallic function of the catalyst, as the formation of hot spots is avoided.

18/00071 Applications of RBI on leakage risk assessment of direct coal liquefaction process
Dou, Z. *et al. Journal of Loss Prevention in the Process Industries*, 2017, 45, 194–202.
Direct coal liquefaction process is the core of coal-to-liquids manufacturing. Due to the strict operating conditions and quantities of hazardous materials involving in the process, conceivable occurrence of leaking may lead to devastating accidents. In this paper, the risk-based inspection (RBI) technique is introduced to be applied in the leakage risk assessment of direct coal liquefaction process. According to the on-site investigation, four leakages rooted in abrasion, untightened seals, fatigue damage and cracks are determined. The hazardous materials potentially participating in the distinctive leakages consist of dry gas, hydrogen, hydrogen sulfide, sulfur, pulverized coal and liquefied light and heavy oil. Concerning the different occurrence probabilities and consequences of leakage, risk assessment and classification have been performed at all critical locations along process of direct coal liquefaction. Therewith, the corresponding scenarios and outcomes of leakage are determined, and accordingly detecting scheme and methods are proposed. The implementation of leakage risk assessment reinforces the inherently safer design of direct coal liquefaction process.

18/00072 Coke oven gas to methanol process integrated with CO_2 recycle for high energy efficiency, economic benefits and low emissions
Gong, M.-h. *et al. Energy Conversion and Management*, 2017, 133, 318–331.
A process of CO_2 recycle to supply carbon for assisting with coke oven gas to methanol process is proposed to realize clean and efficient coke oven gas utilization. Two CO_2 recycle schemes with respect to coke oven gas, namely with and without H_2 separation before reforming, are developed. It is revealed that the process with H_2 separation is more beneficial to element and energy efficiency improvement, and it also presents a better techno-economic performance in comparison with the conventional coke oven gas to methanol process. The exergy efficiency,

direct CO_2 emission, and internal rate of return of the process with H_2 separation are 73.9%, 0.69 t/t-methanol, and 35.1%, respectively. This excellent performance implies that reforming technology selection, H_2 utilization efficiency, and CO_2 recycle ways have important influences on the performance of the coke oven gas to methanol process. The findings of this study represent significant progress for future improvements of the coke oven gas to methanol process, especially CO_2 conversion integrated with coke oven gas utilization in the coking industry.

18/00073 Maximum combustion temperature for coal-water slurry containing petrochemicals

Strizhak, P. A. and Vershinina, K. Y. *Energy*, 2017, 120, 34–46.

This study examines the temperature change of droplets of coal–water slurry containing petrochemicals (CWSP). The slurry consists of coal and oil processing waste. The temperature of oxidant in a modelled combustion chamber is varied between 600 and 1200 K. The initial size (radius) of CWSP droplets varied in the range of 0.5–3 mm. The study identifies typical temperature trends at the centre and on the surface of the CWSP droplet. The temperature trends represent the following stages: (i) heating of fuel, (ii) evaporation of water and a liquid combustible component, (iii) thermal decomposition of coal and yield of volatiles, (iv) gas phase ignition of volatiles together with vapour of the combustible liquid and (v) heterogeneous ignition of carbon and its burnout. Moreover, these trends indicate the maximum combustion temperatures of CWSP that reflect corresponding heat release. The study specifies the parameters which influence the maximum combustion temperature: fuel component composition, properties of components, droplet size, and the oxidant temperature. Finally, the study defines the minimum ignition temperatures and delay times of sustainable combustion initiation that characterize the ignition inertia. The knowledge of influence of these factors will allow one to predict the optimal conditions for the combustion of the CWSP.

18/00074 Optical experimental study on the characteristics of impinging coal-water slurry flame in an opposed multi-burner gasifier

Song, X. *et al. Fuel*, 2017, 188, 132–139.

Impinging flames have been used for a wide variety of industrial processes, especially for opposed entrained-flow gasification technology. The effective monitoring and controlling of flames are at the core of achieving high energy efficiency, reliable diagnosis for the gasification process and optimal gasification technology. Using an emission spectral analysis of an impinging area during coal-water slurry (CWS) gasification in a lab-scale opposed multi-burner (OMB) gasifier, the criterion for dominant reactions was identified. There were obvious radical emissions in the impinging area, including OH*, H*, NO*, CO_2*, Na* and K* emissions. Intense black-body radiation appeared where the wavelength was longer than 400 nm. The radical emissions showed non-linear variation with O/C, and there was a maximal value at the certain O/C, in accordance with the change of atmosphere, which could serve as a criterion for dominant reactions in gasification. The change tendency of OH* intensity on different conditions at the burner plane was similar to those of temperature and CO_2 concentration. The temperature of the burner plane was the lowest in the reaction area. The change tendency of H* was similar to that of OH*, and there was a linear correlation between OH*/H* and O/C.

18/00075 Production of liquid fuels and activated carbons from fish waste

Fadhil, A. B. *et al. Fuel*, 2017, 187, 435–445.

In this research work, liquid bio-fuels and activated carbons were produced from one non-edible feedstock, fish waste. First, the fish oil was extracted from fish waste and transesterified with methanol and ethanol to produce methylic and ethylic biodiesels, respectively using potassium hydroxide as base catalyst. The fuel properties of the obtained biodiesels met the specifications stipulated by ASTM D 6751. Therefore, waste fish oil can be utilized as a potential non-edible feedstock for biodiesel production. The de-oiled fish was pyrolysed in a laboratory scale fixed bed reactor to produce bio-oil and bio-char. The influence of the pyrolysis temperature, pyrolysis time and particle size of the precursor on the bio-oil yield was investigated. The maximum bio-oil yield of 57.13% w/w was produced at a pyrolysis temperature of 500 °C, 60 min pyrolysis time and particle size of 0.25 mm. The chemical composition of the bio-oil was studied using the elemental analysis, column chromatography, FTIR spectroscopy and ^{1}H NMR spectroscopy. The physical and chemical properties of the bio-fuel obtained were determined and found close to those of bio-oils published in literature. It was concluded that de-oiled fish waste bio-oil can be potentially utilized as a fuel and chemical feedstock. The bio-char obtained as a result of the pyrolysis of de-oiled fish waste at 500 °C was used in the preparation of the activated carbon via steam activation method. The influence of the activation temperature, activation time and particles size on the yield, iodine adsorption number and surface area of the produced activated carbons were investigated. The optimal conditions which gave the best activated carbon sample were 500 °C activation temperature, 60 min activation time and 60 mesh particle size. The produced activated carbon was also analysed for its morphology using scanning electron microscope, which indicated that the produced activated carbon has various pore size distribution.

18/00076 Study on saccharification techniques of alga waste harvested from a eutrophic water body for the transformation of ethanol

Chen, S.-T. *et al. Renewable Energy*, 2017, 101, 311–315.

Given the increasing number of cases of water eutrophication and large quantities of naturally grown algae, this study collected algae for bioethanol production from a eutrophic water body. The compositions of alga biomass collected from the eutrophic water body are more complicated than pure culture. The saccharification technique is also different from the conventional one. This study applied an electro-coagulation/flotation (ECF) system to recycle eutrophic algae. After a pre-treatment processes, this study investigated three types of algal biomass to determine the optimal conditions for acid saccharification: Al-containing algal biomass (S1), Fe-containing algal biomass (S2) and raw algal biomass (S3). The results revealed that S1 and S3 attained the highest reducing sugar yields after a 30-min reaction under the following conditions: sulfuric acid concentration = 6% (V/V), liquid–solid ratio (LSR) = 26 and temperature = 120 °C. The maximum reducing sugar yield from S2 occurred at a LSR of 22, yielding up to 156 mg glucose/g and achieving a xylose yield that is twice higher than the glucose yield. Therefore, adopting an ECF system with a Fe electrode for recycling algae advances current research on the saccharification of algae. Recently, the proposed technique has been approved as a new patent by the Taiwanese government.

18/00077 Techno-economic analysis of production of Fischer-Tropsch liquids via biomass gasification: the effects of Fischer-Tropsch catalysts and natural gas co-feeding

Rafati, M. *et al. Energy Conversion and Management*, 2017, 133, 153–166.

The effects of H_2/CO ratio in syngas from a biomass gasifier, the type of a Fischer–Tropsch (FT) catalyst, addition of a reformer in a recycle mode, efficiency of CO_2 removal, and co-feeding of biomass and natural gas on the overall thermal efficiency and costs for the production of FT liquid fuels from the biomass-derived syngas were analysed using an Aspen Plus-based process model. The overall thermal efficiency for biomass-fed processes was in a range of 41.3–45.5%. A cobalt catalyst-based FT process achieved slightly higher efficiency than an iron-based FT process mainly owing to the absence of water–gas shift activity on a cobalt FT catalyst. A proper amount of CO_2 in the syngas can inhibit the amount of CO_2 generated via the water–gas shift reaction in a FT reactor with an iron-based catalyst which yields a similar efficiency to a cobalt-based FT process. The lowest production costs were around $28.8 per GJ of FT liquids for the biomass fed processes with a reformer. However, the addition of a reformer in the gas recycle loop can improve the economics only when the operation of the plant is optimized for maximum fuel production rather than co-generation of fuels and power. A process with co-feeding of natural gas into the reformer can achieve more attractive economics than a solely biomass fed process. Co-feeding of biomass and natural gas each at 200 MW_{th} for a total feedstock thermal energy input of 400 MW_{th} reduced the costs of FT liquid production by about 30% to $19–$20 per GJ of FT liquids. However, production of FT biofuels would be economically viable only at very high oil price or if some premiums are considered for the production of green fuels and power. At an oil price of $60/barrel, production of FT biofuels in the process configurations considered in this study would not be economically feasible.

03 GASEOUS FUELS

Sources, properties, recovery, treatment

18/00078 An approach to estimate gas hydrate saturation from 3-D heterogeneous resistivity model: a study from Krishna-Godavari basin, Eastern Indian offshore

Jana, S. *et al. Marine and Petroleum Geology*, 2017, 79, 99–107.

A method is proposed to estimate gas hydrate saturation from three-dimensional (3-D) heterogeneous model of resistivity simulated using resistivity log. Pure gas hydrates are highly resistive compared to the host sediments, and their presence in the pore space of sediments

increase the resistivity of the formation. The anomalous increase of resistivity is used as a proxy for the delineation of gas hydrates using the resistivity log. A 3-D heterogeneous resistivity model has been constructed from one dimensional resistivity log in the Krishna Godavari basin, eastern Indian offshore. The simulated model contains all small-scale variation in resistivity of the reservoir and maintains all properties associated with covariance, like root mean square fluctuation, characteristic scales and fractal dimension of the observed log. The authors have estimated volumetric hydrate saturation using the three dimensional simulated model. The porosity used for estimating hydrate saturation is calculated from the simulated density field generated using the observed density log. Estimated average gas hydrate saturation is about 9.84% of the pore volume over a 1000 m × 1000 m × 131 m volume.

18/00079 Application of AVO attribute inversion technology to gas hydrate identification in the Shenhu area, South China Sea

Wang, X. and Pan, D. *Marine and Petroleum Geology*, 2017, 80, 23–31.

Amplitude versus offset (AVO) is a seismic exploration technology applied to recognize lithology and detect oil and gas through analysing the feature of amplitude variation versus offset. Gas hydrate and free gas can cause obvious AVO anomaly. To find geophysical evidence of gas hydrate and free gas in Shenhu Area, South China Sea, AVO attribute inversion method is applied. By using the method, the multiple seismic attribute profiles and AVO intercept versus gradient cross plot are obtained. Bottom-simulating reflector (BSR) is observed beneath the seafloor, and the AVO abnormal responses reveal various seismic indicators of gas hydrate and free gas. The final AVO analysis results indicate the existence of gas hydrate and free gas in the upper and lower layers of BSR in the study area.

18/00080 Characteristics and origin of in-situ gas desorption of the Cambrian Shuijingtuo Formation shale gas reservoir in the Sichuan Basin, China

Tang, X. *et al. Fuel*, 2017, 187, 285–295.

In situ shale gas extraction provides direct evidence in response to gas-bearing evaluations and productivity predictions regarding shale gas reservoirs. The desorption characteristics and origin of *in situ* shale gas extraction in the lower Cambrian Shuijingtuo Formation of the Sichuan Basin are studied via *in situ* gas desorption tests. Tests are conducted at both reservoir (35 °C) and high temperatures (90 °C). The results indicate that most *in situ* shale gas is quickly desorbed within 300 min at both the reservoir temperature desorption stage and the high temperature desorption stage. In both instances, the *in situ* gas desorption rates decrease rapidly over time. In addition, the desorbed gas content and desorption rate at the reservoir temperature desorption stage are both clearly lower than the equivalent measures at the high temperature desorption stage. The *in situ* desorbed gas from the reservoir temperature desorption stage is mainly free gas; the *in situ* desorbed gas from the high temperature desorption stage, on the other hand, is mainly sorbed gas, which is the dominant form in the *in situ* shale gas. The percentage of *in situ* desorbed gas at these two stages is mainly controlled by gas adsorption, pore volume, and specific surface area. The desorption rate of *in situ* shale gas is likely controlled primarily by average pore size and methane adsorption.

18/00081 Evaluation of the shale gas potential of the lower Silurian Longmaxi Formation in northwest Hunan Province, China

Wan, Y. *et al. Marine and Petroleum Geology*, 2017, 79, 159–175.

Commercial gas production has been achieved in China's marine shale of the Silurian Longmaxi formation in the eastern Sichuan area, and experience for developing shale gas in complex structural areas has been gathered. A set of Longmaxi Formation shales deposited in the north-western Hunan area has close relationship with the eastern Sichuan Longmaxi shale on both depositional environment and tectonic evolution. Therefore, it is important to undertake an integrated evaluation of the Longmaxi formation shale in the north-western Hunan area. This work combined field investigations and the laboratory measurements using outcrop samples to study the petrology, geochemistry, reservoir and adsorption characteristics of the Longmaxi shale in the north-western Hunan area. The geological settings and reservoir properties were compared with those of the eastern Sichuan Longmaxi shale using publically available data. The results show that the hydrocarbon generation ability, organic matter maturity, sealing capacity and reservoir stimulation effectiveness of the Longmaxi Formation shale in the northwestern Hunan area are comparable to those in the eastern Sichuan area. The Longmaxi shale in the northwestern Hunan area therefore shows early signs of development potential, and the drilling of exploration wells is thus warranted to further evaluate its gas content and other *in situ* reservoir properties for possible shale gas development in the near future.

18/00082 Experimental study on ceiling gas temperature and flame performances of two buoyancy-controlled propane burners located in a tunnel

Wan, H. *et al. Applied Energy*, 2017, 185, 573–581.

Multiple energy sources in a tunnel might lead to merge of flames with small enough spacings, releasing more heat and pollutant emissions than a single energy release source in tunnel and thus posing a great threat to tunnel structure, facilities and trapped people. As the heat detection, controlling and cooling systems are originally designed for the single energy release source, while the spacing between energy sources in tunnel is changeable and unpredictable. Then it is important and helpful to research on the much different characteristics of multiple energy sources with interacting ceiling flames for effective control the high risk scenarios. This paper aims to study the ceiling gas temperature profile and flame properties induced by two interacting energy sources in tunnel so as to improve the understanding of the arrangement of heat detectors and water sprinklers in tunnel. Two identical propane burners were used as energy sources located in a longitudinal array in tunnel. The total energy release rate and burner spacing were varied. The flame merging probability, ceiling gas temperature, vertical flame height and longitudinal flame extension were measured. The criteria of beginning merging and fully merging of flames are respectively proposed for two energy sources in tunnel. Results showed that the area of ceiling flame region increases with higher energy release rate. Models for predicting the ceiling gas temperature profiles induced by two energy sources in tunnel are established respectively for weak and strong plumes impinging on the ceiling. A modified model for predicting the combined vertical and longitudinal flame lengths from two burners in tunnel is proposed involving the normalized energy release rate, burner size and spacing. Finally, the comparison between models proposed for ceiling gas temperatures and flame lengths in tunnel and other configurations identifies the high risk of multiple energy sources in tunnel.

18/00083 Geochemical characteristics of tight gas and gas-source correlation in the Daniudi gas field, the Ordos Basin, China

Wu, X. *et al. Marine and Petroleum Geology*, 2017, 79, 412–425.

The molecular composition, stable carbon and hydrogen isotopes and light hydrocarbons of the Upper Paleozoic tight gas in the Daniudi gas field in the Ordos Basin were investigated to study the geochemical characteristics. Tight gas in the Daniudi gas field displays a dryness coefficient (C_1/C_{1-5}) of 0.845–0.977 with generally positive carbon and hydrogen isotopic series, and the C_7 and C_{5-7} light hydrocarbons of tight gas are dominated by methylcyclohexane and iso-alkanes, respectively. The identification of gas origin and gas-source correlation indicate that tight gas is coal-type gas, and the gases reservoired in the Lower Permian Shanxi Fm. (P_1s) and Lower Shihezi Fm. (P_1x) had a good affinity and were derived from the P_1s coal-measure source rocks, whereas the gas reservoired in the Upper Carboniferous Taiyuan Fm. (C_3t) was derived from the C_3t coal-measure source rocks. The molecular and methane carbon isotopic fractionations of natural gas support that the P_1x gas was derived from the P_1s source rocks. The differences of geochemical characteristics of the C_3t gas from different areas in the field suggest the effect of maturity difference of the source rocks rather than the diffusive migration, and the large-scale lateral migration of the C_3t gas seems unlikely. Comparative study indicates that the differences of the geochemical characteristics of the P_1s gases from the Yulin and Daniudi gas fields originated likely from the maturity difference of the *in situ* source rocks, rather than the effect of large-scale lateral migration of the P_1s gases.

18/00084 Hot spot hunting: optimising the staged development of shale plays

Willigers, B. J. A. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 553–563.

The development of unconventional plays tends to unfold in many stages, each of which involves incremental investment and a reduction in the geological uncertainty of the reservoir. These two characteristics yield a large decision space where future decisions are optimized based on the near-continuous arrival of new information. This managerial flexibility can be exploited by operators during the development of unconventional plays. This study introduces a methodology that demonstrates how value can be created by a staged and partial development of a shale play that would have been unprofitable if fully developed. Compared to existing methods the novel methodology is more consistent with the characteristics of how plays are currently developed as existing methods assume that upon a successful appraisal stage a play is developed in its entirety in a single development phase. As more data become available after each development phase of the play, the potential of the remaining undrilled locations is updated using Bayes's rule. The method is couched in geostatistical principles, combined with an algorithm that allows for a continuous optimization of drilling targets. An example of a shale gas project has been investigated that consists of 225 possible drilling targets each contain-

ing 10 well locations. A maximum of 200 wells can be produced by drilling 20 of the 225 targets. The mean performance of the well population is uncertain. The scenario with the highest mean well performance yields a value of −160 MM US$ and the expected project value across all scenarios of mean well performance equals −920 MM US$, given that all 200 wells are drilled at randomly chosen drilling targets. In the model presented in this study the resource can be developed in up to 19 stages upon completion of an appraisal programme. After each development stage an assessment is made where, and if, the next batch of 10 wells should be drilled. This strategy of stage-wise development yields an expected value of 49.2 MM US$. The spatial dependency of well performance enables the algorithm to restrict the development of the play to the most prolific areas. The appraisal programme provides a view on the variability of well performance across the play. A trade off exists between the size, and the consequential accuracy, of the appraisal programme and the cost of appraising. The example illustrates that the expected project value increases from 33.3 MM US$ for an appraisal programme in which two locations were appraised, to a maximum of 49.2 MM US$ after the appraisal of four locations, and subsequently decreases to 29.0 MM US$ after having appraised eight locations. The assumptions around the variability of estimated ultimate recovery used in this example were informed by data from 10,000 horizontal wells located in the Mississippian Barnett Shale in the Fort Worth basin in Texas.

18/00085 Impact of total organic carbon and specific surface area on the adsorption capacity in Horn River shale

Kim, J. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 331–339.

Among unconventional gas reservoirs, shale gas has become an increasingly important source of natural gas supply in North America and around the world. Horizontal drilling and multi-stage hydraulic fracturing are the two key technologies for the economic development of shale gas reservoirs. Generally, natural gas in shale reservoirs is stored as free gas state in both larger mineral pores and natural fractures, as well as adsorbed gas state within organic matter and clay minerals. Since a considerable fraction of the gas in place (GIP) is in the adsorbed state, investigation of gas adsorption can provide critical insights into the evaluation of resources volume in shale. In this study, several experiments are carried out on 14 shale core samples obtained in a vertical well drilled in Horn River Basin, Canada. The total organic carbon (TOC) content, specific surface area (SSA), and CH_4 adsorption isotherm are measured for the samples. In order to measure the volume of adsorbed gas at reservoir pressure, the high pressure Belsorp-HP equipment applying volumetric method is used. As results, it is observed that adsorption capacity is a function of not only the TOC but also the SSA. When the samples have similar TOC, adsorption capacity becomes higher as SSA increases and Langmuir volume increases too. The authors also consider the relationship between SSA and adsorption capacity for each kerogen quality that it shows a linear trend. Also, the authors attempt to find a correlation of TOC and SSA to the adsorption capacity by categorizing experimental results. Finally, gas in place calculation is carried out for the free gas and adsorbed gas in Horn River shale, respectively.

18/00086 Influence of coal petrology on methane adsorption capacity of the Middle Jurassic coal in the Yuqia Coalfield, northern Qaidam Basin, China

Hou, H. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 218–227.

The lower coalbed methane (CBM) adsorption capacity of the low rank coals is not only related to its lower maturity, but also determined by the coal maceral compositions. In this study, a total of 13 samples including 10 coals and 3 carbonaceous mudstones, were collected from the Middle Jurassic Dameigou Formation in the borehole YQ-1 of the Yuqia Coalfield, northern Qaidam Basin, NW China. Coal lithotypes, maceral compositions, coal ranks, coal facies and methane adsorption characteristics of these samples were investigated using microscopic observation, proximate analysis, porosity analysis, and isothermal adsorption experiments. The results show that the maceral composition has a great influence on the methane adsorption capacity, and the influence of vitrinite on the methane adsorption is generally stronger than that of inertinite at a similar coal rank. For most samples, there is a positive correlation between the vitrinite contents and the Langmuir volume (V_L), a negative correlation between the inertinite contents and the V_L, and no obvious correlation between the exinite contents and the V_L. Furthermore, the vitrinite/inertinite (V/I) ratio also shows a positive relationship with the V_L. However, some samples containing large amounts of unfilled fusinite and/or semifusinite have more pore spaces favouring methane adsorption and can also adsorb significant quantities of methane. Consequently, coals with higher vitrinite contents, in association with some unfilled fusinites or semifusinites, should have the greatest adsorption capacity. Coal maceral compositions vary with the types of coal facies, and thus the methane adsorption capacity of coals may be closely related to coal facies. It is found that the methane adsorption capacities of the coals in a wet forest swamp (Type I) and an intergradation forest swamp (Type II) are greater than those in a drained forest swamp (Type III) and an open water peat swamp (Type IV). It is suggested that the area developed with the wet forest swamp and in the intergradation forest swamp with high porosity should be the best target areas for the CBM exploration in the Yuqia Coalfield.

18/00087 Inhibiting effects of nitrogen compounds on deep hydrodesulfurization of straight-run gas oil over a NiW/Al_2O_3 catalyst

Tao, X. *et al. Fuel*, 2017, 188, 401–407.

The inhibiting effects of nitrogen compounds on the hydrodesulfurization (HDS) of thiophene-series sulfur compounds in straight-run gas oil over a NiW/Al_2O_3 catalyst were studied. The nitrogen compounds investigated here were quinoline and indole; nitrogen to sulfur mass ratios (N/S) varying from 0.9 to 1.2 were comparably studied. The results showed that quinoline was much easier to be converted but harder to be denitrogenated as compared with indole. Quinoline displayed stronger inhibiting effects on the HDS of individual sulfur compounds in the gas oil than that of indole. Langmuir–Hinshelwood type rate equations were used to compare the nitrogen inhibiting effects. The nitrogen inhibiting effects on these thiophene series sulfur compounds decreased in the order 4,6-DMDBT(4,6-dimethyl-dibenzothiophene) > 4-MDBT > C1DBT > DBT > C2-C3DBT. The HDS of C2-C3DBT group with relative substituents at different four and six positions got the lowest nitrogen inhibiting effects due to their better approach abilities to the catalyst.

18/00088 Interactions between coal seam gas drainage boreholes and the impact of such on borehole patterns

Liu, Z. *et al. Journal of Natural Gas Science and Engineering*, 2017, 38, 597–607.

Borehole drainage is the most effective means of extracting coal seam gas. However, numerous boreholes are usually needed to create strong drainage from a single coal seam. When multiple boreholes work at the same time, borehole interactions will occur, which strongly affect the gas production and the area controlled by each borehole. To accurately quantify the degree of interaction, this paper utilizes the changes in the gas pressure at points around the borehole to calculate the pressure decrease coefficients, which reflect the degree of disturbance between the boreholes. The relationships between the physical parameters of the coal seam and the pressure decrease coefficients are studied with a typical double borehole interaction model. The results illustrate that the pressure decrease coefficients are positively correlated with the coal permeability in the disturbance region. Furthermore, the relation between the pressure decrease coefficients and borehole separation forms a negative exponential function, whereas the relation between the pressure decrease coefficients and the distance from the borehole forms a positive index function. Multi-borehole patterns are also analysed to investigate the ability of the pressure decrease coefficients to determine which common borehole pattern is most suitable for efficient gas extraction.

18/00089 Maximization of energy recovery inside supersonic separator in the presence of condensation and normal shock wave

Shooshtari, S. H. R. and Shahsavand, A. *Energy*, 2017, 120, 153–163.

Natural gases provide around a quarter of energy consumptions around the globe. Supersonic separators (3S) play multifaceted role in natural gas industry processing, especially for water and hydrocarbon dew point corrections. These states of the art devices have minimum energy requirement and favourable process economy compared to conventional facilities. Their relatively large pressure drops may limit their application in some situations. To maximize the energy recovery of the dew point correction facility, the pressure loss across the 3S unit should be minimized. The optimal structure of 3s unit (including shock wave location and diffuser angle) is selected using simultaneous combination of normal shock occurrence and condensation in the presence of nucleation and growth processes. The condense-free gas enters the non-isentropic normal shock wave. The simulation results indicate that the normal shock location, pressure recovery coefficient and onset position strongly vary up to a certain diffuser angle ($\beta = 8°$) with the maximum pressure recovery of 0.88 which leads to minimum potential energy loss. Computational fluid dynamic simulations show that separation of boundary layer does not happen for the computed optimal value of β and it is essentially constant when the inlet gas temperatures and pressures vary over a relatively broad range.

18/00090 New forecasting method for liquid rich shale gas condensate reservoirs with data driven approach using principal component analysis

Khanal, A. *et al. Journal of Natural Gas Science and Engineering*, 2017, 38, 621–637.

Accurate production performance evaluation and forecasting in shales during the early stages of development can play an important role in minimizing uncertainties associated with unconventional reservoirs. Given the limited reliability in forecasts from traditional decline models when applied to unconventional reservoirs, new tools to supplement the ones in use today are required to improve the accuracy of production forecasts. This study presents a method involving principal component analysis (PCA), which is a simple, non-parametric method of extracting relevant information from large data sets to perform production forecasting of liquid rich shale gas condensate reservoirs. The authors used a comprehensive compositional reservoir model to create several iterations of synthetic production histories from liquid rich shales (LRS) wells based on Monte Carlo simulation with predefined probability distributions. Cumulative gas, gas rate, and condensate-to-gas ratio (CGR) for the simulated cases were decomposed into principal component (PC) scores and coefficients were used to recreate the original data. The dataset was cross-validated to check its ability to predict the missing production data based on PC scores and coefficients of the limited production data. Principal component analysis was further applied to the field data from several wells from Eagle Ford shale. The authors re-created and cross-validated the field data by using limited PC which led to good matches of the original production data. Two to three PCs were required to recreate the initial data with reasonable accuracy depending on the quality of the input data. During the validation step, it was observed that some of the wells exhibited significant error which could be attributed to significantly different production profiles of those wells compared to the other wells. For simulated data, four PC was enough to yield the prediction with average error of 0.16%, 0% and 0.77% respectively for gas rate, cumulative gas and CGR respectively. For field data, three PC yielded the best prediction with average error of 1.63% and 2.98% for gas rate and oil rate respectively. This work shows that multivariate statistics and data driven methods can be used as an important approach to complement existing tools like reservoir simulation and decline curve analysis to perform production data analysis. PCA can also be used and can generate accurate results relatively quickly. It was recognized that even more rapid approximate methods will be required for routine analysis. Understanding the limitations of different approximate methods and application of methods to overcome these limitations in given circumstances should lead to optimal use of these methods.

18/00091 Petroleum accumulation in the deeply buried reservoirs in the northern Dongying Depression, Bohai Bay Basin, China: new insights from fluid inclusions, natural gas geochemistry, and 1-D basin modeling

Ping, H. *et al. Marine and Petroleum Geology*, 2017, 80, 70–93.

The deeply buried reservoirs (DBRs) from the Lijin, Shengtuo and Minfeng areas in the northern Dongying Depression of the Bohai Bay Basin, China exhibit various petroleum types (black oil-gas condensates) and pressure systems (normal pressure–overpressure) with high reservoir temperatures (154–185 °C). The pressure-volume-temperature-composition (PVTX) evolution of petroleum and the processes of petroleum accumulation were reconstructed using integrated data from fluid inclusions, stable carbon isotope data of natural gas and one-dimensional basin modelling to trace the petroleum accumulation histories. The results suggest that (1) the gas condensates in the Lijin area originated from the thermal cracking of highly mature kerogen in deeper formations. Two episodes of gas condensate charging, which were evidenced by the trapping of non-fluorescent gas condensate inclusions, occurred between 29–25.5 Ma and 8.6–5.0 Ma with strong overpressure (pressure coefficient, $P_c = 1.68–1.70$), resulting in the greatest contribution to the present-day gas condensate accumulation; (2) the early yellow fluorescent oil charge was responsible for the present-day black oil accumulation in well T764, while the late blue-white oil charge together with the latest kerogen cracked gas injection resulted in the present-day volatile oil accumulation in well T765; and (3) the various fluorescent colours (yellow, blue-white and blue) and the degree of bubble filling (F_v) (2.3–72.5%) of the oil inclusions in the Minfeng area show a wide range of thermal maturity (API gravity ranges from 30° to 50°), representing the charging of black oil to gas condensates. The presence of abundant blue-white fluorescent oil inclusions with high Grain-obtaining Oil Inclusion (GOI) values (35.8%, usually >5% in oil reservoirs) indicate that a paleo-oil accumulation with an approximate API gravity of 39–40° could have occurred before 25 Ma, and gas from oil cracking in deeper formations was injected into the paleo-oil reservoir from 2.8 Ma to 0 Ma, resulting in the present-day gas condensate oil accumulation. This oil and gas accumulation model results in three oil and gas distribution zones: (1) normal oil reservoirs at relatively shallow depth; (2) gas condensate reservoirs that originated from the mixture of oil cracking gas with a paleo-oil reservoir at intermediate depth and (3) oil-cracked gas reservoirs at deeper depth. The retardation of organic matter maturation and oil cracking by high overpressure could have played an important role in the distribution of different origins of gas condensate accumulations in the Lijin and Minfeng areas. The application of oil and gas accumulation models in this study is not limited to the Dongying Depression and can be applied to other overpressured rift basins.

18/00092 The situation analysis of shale gas development in China – based on structural equation modeling

Ma, Z. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 1300–1307.

Shale gas is a significant source of unconventional energy. With the largest recoverable reserves in the world, China has 36.1 trillion cubic metres of shale gas, which will contribute to ensuring its national energy security and promoting the diversity of energy supply. Chinese government spares no effort to support the utilization and development of shale gas. However, the development of shale gas remains deeply troubled; thus the authors would like to reveal the factors influencing shale gas development in China. Through the study of various literature and carrying out interviews with experts about shale gas development, the authors collected 206 valid questionnaires from experts, scholars or researchers in shale gas field and then used structural equation modelling to analyse the data, illustrate the relationships among environment, technology, resource, market and shale gas development and finally establish a shale gas development implementation model. The research findings would help Chinese government advance shale gas development, and improve further studies in shale gas area.

18/00093 Tomographic absorption spectroscopy for the study of gas dynamics and reactive flows

Cai, W. and Kaminski, C. F. *Progress in Energy and Combustion Science*, 2017, 59, 1–31.

Optical imaging techniques are ubiquitous for the resolution of non-uniformities in gas flows. Planar imaging techniques such as laser-induced fluorescence are well established and applied extensively in turbulent reactive flows, offering both high temporal and spatial resolutions. However, planar imaging suffers from a critical disadvantage, the requirement for spatially continuous optical access over large solid angles in both the excitation and detection paths and this precludes their application in many practical situations, for example those encountered in engine testing. Tomographic absorption spectroscopy, TAS, on the other hand, shares many of the advantages of planar imaging techniques but reduces the demands for optical access, because high quality data can be obtained with sparsely sampled volumes. The technique has unrivalled potential for imaging in harsh environments, for example for in-cylinder/in-chamber engine measurements. TAS is beginning to mature as a technique for the simultaneous imaging of temperature and species concentration, and is experiencing a surge of interest due to progress in laser technology, spectroscopy, and theoretical developments of non-linear tomography techniques. The recent advancements in broad bandwidth, frequency-agile laser sources massively enrich the spectral information obtainable in TAS. Furthermore, non-linear tomography enables the recovery of multiplexed information from a single tomographic inversion. The utilization of multispectral information improves the immunity of TAS to experimental noise and makes possible the simultaneous imaging of temperature, pressure, and multiple species. Non-linear tomography can also be used to empower the imaging potential of sensitive and robust absorption techniques, such as wavelength modulation spectroscopy, for use in harsh and even optically dense environments. In combination, this greatly extends the applicability of TAS for more general and harsh scenarios in combustion technology. This paper reviews basic concepts and mathematical foundations of classical absorption tomography, proceeding to more advanced recent concepts based on non-linear tomography, and providing an extensive review of experimental demonstrations and practical applications in the context of state-of-the-art combustion research.

Transport, storage

18/00094 Application of PSO and cultural algorithms for transient analysis of natural gas pipeline

Madoliat, R. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 504–514.

System simulation is an essential step for the optimization and control of natural gas transmission networks. Transient simulation of natural gas networks is more accurate than steady state simulation, but it imposes the complexity of solving non-linear PDE flow equations. In this paper, a novel approach based on using two meta-heuristic algorithms: (a) particle swarm optimization (PSO), (b) cultural algorithm (CA) is presented to simplify transient simulation of gas networks with known inlet and outlet pressures. PSO or CA estimates different values for the network inlet flow rates. Using each of these

estimated values, both boundary conditions will be known at the network inlets and discretized flow equations can be linearized. These linear flow equations will be solved for the network inlet nodes. This procedure will be continued for the next nodes until reaching network outlets. Then the differences of calculated and actual network outlet pressures will be defined as a cost function or error. Eventually, these algorithms will obtain the optimum inlet flow rates which minimize the cost function. Thus, the calculated pressures and flow rates at different gas network nodes which are obtained by using these optimum inlet flow rates will be the true values. The proposed approach reduces the complexity of solving network transient flow equations with the mentioned boundary conditions while simulation results confirm its accuracy and efficiency.

18/00095 CFD prediction of Black Powder particles' deposition in vertical and horizontal gas pipelines

Kharoua, N. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 822–833.

The deposition of Black Powder particles in gas pipelines is a critical industrial problem. Gas-solid flow in a pipe is simulated using the Reynolds stress model (RSM) and the Discrete Phase Model (DPM). In this study, 3D meshes for pipes with different orientations are considered. Vertical orientations were, also, considered although they are not as common as the horizontal pipeline in the gas industry. Efforts were made to predict an accurate turbulent flow field as a requirement for successful simulation of particle deposition velocity. A fine mesh was used to resolve the viscous sublayer and DNS or experimental profiles of the fluctuating velocities were imposed to minimize the inaccurate prediction of the RSM model to determine the fluctuating velocity needed for the particle trajectories. Black Powder particles, in the range 1–50 μm, were injected in the computational domain as mono-dispersed and poly-dispersed size distributions respectively. The spatial distribution of the particles, injected at the inlet of the three-dimensional pipe, was randomly varied with time to replicate realistic distributions. The predicted deposition velocity, presented a relatively good agreement with benchmark experiments from the literature. The trends of the deposition velocity curve in horizontal and vertical pipes are different. Ascending and descending vertical flows yield similar deposition velocity curves. In addition, the concentration decay was also obtained in order to determine the approximate distances that particles, with different diameters, can reach in pipelines.

18/00096 Comprehensive risk evaluation of underground energy storage caverns in bedded rock salt

Zhang, N. *et al. Journal of Loss Prevention in the Process Industries*, 2017, 45, 264–276.

Rock salt is accepted as an ideal medium for underground energy storage due to its low permeability, favourable creep and damage recovery properties. Different from the 'pure' salt domes in Europe and other western countries, bedded salt deposits with multiple thin interlayers buried at shallow depth are widespread in China. The complex geological conditions increase the risk possibility of underground energy storage disaster. The comprehensive risk evaluation is of great importance for underground energy storage in bedded rock salt. According to the statistical results of catastrophic accidents in global rock salt mining, the risk factors leading to the oil or gas leakage, surface subsidence and the cavern group failure were analysed and identified with the fault tree method. On this basis, the performance functions of surrounding rock slabbing, cavern tightness, excessive volume convergence and surface subsidence were proposed. The comprehensive risk probability evaluation methodology and risk classification standard were established for underground bedded rock salt storage cavern. By application of the comprehensive risk assessment system, the risk failure probability for Jintan bedded salt cavern group was calculated and the integrated risk level of which was evaluated. The appropriate operating pressure range (3–22 MPa) determined through theoretical calculation for Jintan bedded salt cavern group at a lower risk level coincides with that obtained from the conducted three-dimensional geomechanical model tests, verifying the validity of the proposed comprehensive risk evaluation method.

18/00097 Effect of long-term operation on steels of main gas pipeline. Reduction of static fracture toughness

Maruschak, P. O. *et al. Journal of Natural Gas Science and Engineering*, 2017, 38, 182–186.

The effect of the long-term operation on changes in the parameters of fracture toughness and a tendency for a delayed fracture of the steel of main gas pipelines is investigated. Based on the method of the full strain diagrams the general regularities of operational degradation influence onto the static fracture toughness and microscale failure mechanisms of 17MnSi steel after long-term operation have been established. Generalization of results on the influence of absorbed hydrogen onto the pipeline steel structure and fracture pattern made possible to systemize the data on dispersed damage accumulation. The schematization of fracture mechanisms of 17MnSi steel is offered. The proposed approaches to the study of static fracture toughness of the steel of the main gas pipelines can be used in the evaluation of their technical conditions and planning of their overhaul.

18/00098 Formation of clathrate cages of sI methane hydrate revealed by *ab initio* study

Liu, J. *et al. Energy*, 2017, 120, 698–704.

Here the authors studied the formation micro-mechanism of the small and large cages in the nucleation pathway of sI methane hydrate using *ab initio* calculations. It was found that the cage precursor is a pentagonal ring of water molecules plus one methane molecule, which is formed through the attraction of the pentagonal water ring to the methane molecule. Due to the difference of the hydrophobic-hydrophilic effects, the ring expansion mechanism and the layer-separated mechanism are observed for the growth of water faces in the small and large cages, respectively. Further, formation of the small cage is more structurally feasible and will locally prefer in the early stage of nucleation, but the large cages will dominate in the crystalline structure of methane hydrate, attributing to their high stabilization energy.

18/00099 Prediction of storage efficiency on CO_2 sequestration in deep saline aquifers using artificial neural network

Kim, Y. *et al. Applied Energy*, 2017, 185, 916–928.

This study presents the application of artificial neural network (ANN) to predict storage efficiency of CO_2 sequestration in deep saline aquifers. To a create training database used as input and output neurons in ANN, sensitivity analysis of parameters considering the aquifer characteristics was performed by numerical simulation. Based on the analysis, the factors and their ranges influencing CO_2 sequestration in deep saline aquifers were determined and 150 representative realizations used as a training database were generated with trapping indices of the residual CO_2 and solubility trapping mechanisms. The ANN model was designed with optimum architecture minimizing the mean squared error for testing data set and it was tested with validation samples. The results showed that the proposed ANN model had a high prediction performance with a high coefficient of determination (R^2) of over 0.99 on comparing with the target values, a low mean absolute percentage error (MAPE) of 1.26%, and root mean square error (RMSE) of 0.41 for total trapping efficiency index (TEI). As a field application, the model has also been evaluated with the field scale data on the Gorae V structure in Block VI-1, Korea. The results of prediction were well matched with the targeted values and accuracy between the ANN predictions and field scale data was achieved with a high coefficient of determination (R^2) of more than 0.96, a low MAPE of 4.40%, and RMSE of 3.58 for TEI. From these results, it is believed that the newly developed ANN model can predict storage efficiency with high accuracy and it can also be considered as a useful and robust tool to evaluate the feasibility of CO_2 sequestration in deep saline aquifers.

18/00100 Pressure responses and phase transitions during the release of high pressure CO_2 from a large-scale pipeline

Guo, X. *et al. Energy*, 2017, 118, 1066–1078.

As part of the carbon capture and storage (CCS) process, pipeline transportation is the safest and most economic option for delivering captured CO_2 to a storage site. However, in the event of pipeline rupture an enormous mass of CO_2 may be released very rapidly, presenting several risks to the pipeline and surrounding population including the significantly increased risk of brittle fracture in the pipe wall. The study of pressure variation and phase change in CO_2 during pipeline blowdown can contribute to the understanding of fracture initiation and propagation, as well as downstream CO_2 diffusion behaviour. As part of the CO_2 QUEST project, a reusable, industrial scale pipeline experimental apparatus with a total length of 258 m and the inner diameter of 233 mm was fabricated to study pure CO_2 pipeline blowdown. A dual-disc blasting device was used to remotely control the opening of the pipeline. The instantaneous pressure response following release was measured with high frequency pressure transducers. Variation in fluid temperature at the top and bottom of pipeline was also recorded. Six groups of pure CO_2 pipeline release experiments were conducted with initially gaseous and dense phase inventories with three orifice diameters (15 mm, 50 mm and full bore rupture). The typical waveform characteristics of pressure responses accompanying by the process of phase transitions in gaseous and dense CO_2 leakage were observed during the release as results of the propagation of a series of expansion waves. The complicated phase transitions were obtained during depressurization of gaseous and dense CO_2 releases. The gas-solid phase or gas-liquid-solid phase appeared when the pressure was below the triple point during the dense CO_2 release.

18/00101 Shale-gas wells as virtual storage for supporting intermittent renewables
Knudsen, B. R. and Foss, B. *Energy Policy*, 2017, 102, 142–144.
Mature shale-gas wells possess a property that enables cyclic production and shut-in without incurring revenue losses. Based on this property, it is suggested that fields with mature shale-gas wells may act as virtual gas storage for supplying fast-ramping gas power plants which balance intermittent renewable generation. By enabling gas supply to power plants to circumvent intermediate third-party storage, it is argued that the proposed integration facilitates demand-driven gas production, and discuss how the scheme may support utilization of renewables and reduce supply-related greenhouse-gas emissions in electricity generation.

18/00102 Strength reduction for upheaval buckling of buried pipes in blocky clay backfill
Brennan, A. J. *et al. Ocean Engineering*, 2017, 130, 210–217.
Offshore pipelines are often buried to protect the pipeline from external loads and upheaval buckling. Models for pipe uplift resistance in clay soils are based predominantly on homogenous backfill conditions. In practice, however, there will be significant soil disturbance during installation. With certain trenching techniques this may produce a backfill more akin to a matrix of lumps of intact soil connected by weaker remoulded interfaces. This research uses centrifuge modelling to assess the resistance provided by a representative lumpy clay backfill that has experienced self-weight consolidation. A model pipe is then uplifted through this model backfill in order to assess the soil uplift resistance. Results show that the uplift resistance in this material is governed strongly by the size of the lumps and, to a lesser extent, by the rate at which displacement occurs. When interpreted in terms of the strength reduction η, that may be used to correct between theoretical and measured uplifts, lower values were derived than those currently used based on intact soils. The value of η is seen to be controlled by a non-dimensional drainage parameter, but may be practically estimated based on an estimate of the size of lumps relative to the pipe diameter.

Economics, business, marketing, policy

18/00103 A new approach for the comprehensive grading of petroleum reserves in China: two natural gas examples
Li, W. *et al. Energy*, 2017, 118, 914–926.
For orderly and sustainable development, petroleum resources should be planned scientifically. Based on the discount cash flow method, the authors propose a new approach for the comprehensive grading of petroleum reserves in China because existing reserve classification methods are unable to support the formulation of exploitation planning. This approach combines five factors: economic value, technological progress, subsidy policy, reserve scale and resource risk. Examples show that this approach can be used to grade natural gas resources rapidly and effectively, which is helpful for providing effective guidance for the scientific development of gas resources.

18/00104 Dynamic safety assessment of natural gas stations using Bayesian network
Zarei, E. *et al. Journal of Hazardous Materials*, 2017, 321, 830–840.
Pipelines are one of the most popular and effective ways of transporting hazardous materials, especially natural gas. However, the rapid development of gas pipelines and stations in urban areas has introduced a serious threat to public safety and assets. Although different methods have been developed for risk analysis of gas transportation systems, a comprehensive methodology for risk analysis is still lacking, especially in natural gas stations. The present work is aimed at developing a dynamic and comprehensive quantitative risk analysis (DCQRA) approach for accident scenario and risk modelling of natural gas stations. In this approach, a FMEA is used for hazard analysis while a Bow-tie diagram and Bayesian network are employed to model the worst-case accident scenario and to assess the risks. The results have indicated that the failure of the regulator system was the worst-case accident scenario with the human error as the most contributing factor. Thus, in risk management plan of natural gas stations, priority should be given to the most probable root events and main contribution factors, which have identified in the present study, in order to reduce the occurrence probability of the accident scenarios and thus alleviate the risks.

18/00105 Gas reservoir characteristics of the Lower Gondwana Shales in Raniganj Basin of Eastern India
Mendhe, V. A. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 649–664.
In India, Raniganj basin has become a prime target for shale gas exploration. Investigated shale core samples obtained from nine boreholes during exploratory drilling with laterally varying depth from 11 to 1480 m. A substantial amount of organic matter in shale beds having cumulative thickness of 86, 327 and 126 m are found in Raniganj, Barren Measures and Barakar Formations respectively. The total organic content (TOC) of shales signifies poor to excellent (1.01–12.73 wt%), while the values of S1 and S2 revealed poor to good source rock generation potential, accentuating thermally immature to moderately mature shale reservoir. The various plots like HI vs OI, HI vs TOC, S2 vs TOC, PI vs S1 and S2, implies that studied shales are gas prone containing type II/III and type III kerogen except sample No. 17, which has shown type IV kerogen owing to effects of nearby igneous intrusive. Comparatively less sorption in Raniganj shales reflecting low TOC content, whereas Barren Measures and Barakar shales has moderate sorption capacities controlled by organic matter and clay minerals. Low pressure N_2 adsorption-desorption isotherms are used to categorize pore geometry such as cylindrical, slit-shaped and bottle neck pores in Raniganj, Barren Measures and Barakar shales respectively. Organic content have no significant influence over the surface area, because intensified thermal stress could have caused the destruction of thinner organic pores which reduced the involvement of organic pores in surface area. The pores are classified into four types using scanning electron microscopy taking into account the origin, size and shape of pores, (i) dissolved pores – developed due to the effect of groundwater or de-carbonic acid, (ii) open pores associated with organic matter – formed during thermal cracking of kerogen, (iii) intergranular pores – formed due to incomplete cementation and (iv) micro fractures – owing to tectonic movements or structural activities in the basin. The *in situ* gas content obtained from canister test varies from 1.937 to 2.307, 0.378–3.035 and 0.424–1.937 m^3/t for Raniganj, Barren Measures and Barakar shales, respectively. However, large cumulative thickness, high TOC, moderate sorption capacity, well developed pore geometry and significant surface area encourages the exploration and production development of shale gas in Raniganj basin. The estimated recoverable shale gas resource is 30.76 billion cubic metres (BCM) for Raniganj, 103.76 BCM for Barren Measures and 41.69 BCM for Barakar shales. This study would help the operators to fulfil the gap of lack of adequate knowledge to develop the shale gas play in this basin.

18/00106 How does the U.S. natural gas market react to demand and supply shocks in the crude oil market?
Jadidzadeh, A. and Serletis, A. *Energy Economics*, 2017, 63, 66–74.
This study used monthly data (over the period from January 1976 to December 2012) and a structural VAR model to disentangle demand and supply shocks in the global crude oil market and investigate their effects on the real price of natural gas in the USA. The authors identified the model by assuming that innovations to the real price of crude oil are predetermined with respect to the natural gas market and show that close to 45% of the variation in the real price of natural gas can be attributed to structural supply and demand shocks in the global crude oil market.

18/00107 Mapping gas hydrate and fluid flow indicators and modeling gas hydrate stability zone (GHSZ) in the Ulleung Basin, East (Japan) Sea: potential linkage between the occurrence of mass failures and gas hydrate dissociation
Horozal, S. *et al. Marine and Petroleum Geology*, 2017, 80, 171–191.
The Ulleung Basin, East (Japan) Sea, is well known for the occurrence of submarine slope failures along its entire margins and associated mass-transport deposits (MTDs). Previous studies postulated that gas hydrates which broadly exist in the basin could be related with the failure process. This study identified various features of slope failures on the margins, such as landslide scars, slide/slump bodies, glide planes and MTDs, from a regional multi-channel seismic dataset. Seismic indicators of gas hydrates and associated gas/fluid flow, such as the bottom-simulating reflector (BSR), seismic chimneys, pockmarks, and reflection anomalies, were re-compiled. The gas hydrate occurrence zone (GHOZ) within the slope sediments was defined from the BSR distribution. The BSR is more pronounced along the southwestern slope. Its minimal depth is about 100 m below seafloor (mbsf) at about 300 m below sea-level (mbsl). Gas/fluid flow and seepage structures were present on the seismic data as columnar acoustic-blanking zones varying in width and height from tens to hundreds of meters. They were classified into: (a) buried seismic chimneys (BSC), (b) chimneys with a mound (SCM) and (c) chimneys with a depression/pockmark (SCD) on the seafloor. Reflection anomalies, i.e. enhanced reflections below the BSR and hyperbolic reflections which could indicate the presence of gas, together with pockmarks which are not associated with seismic chimneys, and SCDs are predominant in the western-southwestern margin, while the BSR, BSCs and SCMs are widely distributed in the southern and south-western margins. Calculation of the present-day gas-hydrate stability zone (GHSZ) shows that the base of the GHSZ

(BGHSZ) pinches out at water depths ranging between 180 and 260 mbsl. The occurrence of the uppermost landslide scars which is below about 190 mbsl is close to the range of the GHSZ pinch-out. The depths of the BSR are typically greater than the depths of the BGHSZ on the basin margins which may imply that the GHOZ is not stable. Close correlation between the spatial distribution of landslides, seismic features of free gas, gas/fluid flow and expulsion and the GHSZ may suggest that excess pore-pressure caused by gas hydrate dissociation could have had a role in slope failures.

18/00108 'No shut-off' policies and natural gas consumption

Clark, D. E. *et al. Resource and Energy Economics*, 2017, 48, 19–29.

Many US states have regulations that prevent natural gas utility companies from turning off service to non-paying consumers. The goal of these policies, termed 'no shut-off' (NSO) regulations, is to provide a guaranteed minimum level of residential comfort by reducing the marginal cost of consumption to zero for a period of time. This paper employs a difference-in-difference approach applied to residential US Energy Information Administration data to evaluate whether NSO policies generate higher levels of gas usage. The preferred specifications suggest that activation of a NSO policy increases natural gas consumption by between 4.7–4.8%, resulting in a total increase of between 66 and 67 billion cubic feet of natural gas consumed per winter season in covered states, at a value of as much as $950–970 million annually.

18/00109 Optimal hedging in the US natural gas market: the effect of maturity and cointegration

Ghoddusi, H. and Emamzadehfard, S. *Energy Economics*, 2017, 63, 92–105.

This study uses the US natural gas market as the rich experimental context to test multiple features of hedging performances. First, the authors compared the hedging effectiveness of a single futures contract (i.e. Henry Hub) used for hedging six different physical price positions. Second, they examined the performance of hedging, when one uses a futures contract with time-to-maturity beyond the hedging horizon (i.e. a non-matching hedging strategy). Finally, they quantified the effect of accounting for cointegration and also the time varying volatility in the calculation of optimal hedge ratios. As a robustness check the authors conducted their analysis using both *ex ante* (out of sample) and *ex post* (in sample) methods. The findings suggest that using longer maturity contracts may improve the hedging effectiveness. It was also found that accounting for cointegration and time varying prices has minimal effect on the hedge ratio and hedging effectiveness for almost all physical prices. The findings can inform businesses exposed to commodity price risks in on making better risk-management decisions.

18/00110 Production efficiency of Swedish farm-scale biogas plants

Ahlberg-Eliasson, K. *et al. Biomass and Bioenergy*, 2017, 97, 27–37.

Biogas from agricultural waste streams represents an important way to produce fossil-free energy, allow nutrient recycling and reduce greenhouse gas emissions. However, biogas production from agricultural substrates is currently far from reaching its full potential. In Sweden, the number of biogas plants and their output have increased in recent years, but they are still experiencing harsh economic conditions. A recent evaluation (2010–2015) of 31 farm-scale biogas production facilities in Sweden sought to identify parameters of importance for further positive development. In this paper, data on plant operation, gas yield and digestate quality for 27 of these plants are summarized and statistically analysed to investigate factors that could allow an increase in overall biogas production and in nutrient content in the digestate. The analysis showed that addition of co-substrates to manure results in higher gas production, expressed as both specific methane potential and volumetric gas production, than when manure is the sole substrate. Use of co-substrate was also found to be influential for the nutrient content of the digestate. These observed improvements caused by co-digestion should be considered when subsidy systems for manure-based biogas processes are being created, as they could also improve the economics of biogas production. However, to achieve higher efficiency in existing biogas plants and to improve the situation for future investments, a more detailed, long-term evaluation programme should also be considered.

18/00111 The life cycle greenhouse gas implications of a UK gas supply transformation on a future low carbon electricity sector

Hammond, G. P. and O'Grady, Á. *Energy*, 2017, 118, 937–949.

Natural gas used for power generation will be increasingly sourced from more geographically diverse sites, and unconventional sources such as shale and biomethane, as natural gas reserves diminish. A consequential life cycle approach was employed to examine the implications of an evolving gas supply on the greenhouse gas (GHG) performance of a future UK electricity system. Three gas supply mixes were developed based on supply trends, from present day to the year 2050. The contribution of upstream gas emissions – such as extraction, processing/refining – is not fully reported or covered by UK government legislation. However, upstream gas emissions were seen to be very influential on the future electricity systems analysed; with upstream gas emissions per MJ rising between 2.7 and 3.4 times those of the current supply. Increased biomethane in the gas supply led to a substantial reduction in direct fossil emissions, which was found to be critical in offsetting rising upstream emissions. Accordingly, the modelled high shale gas scenario, with the lowest biomethane adoption; resulted in the highest GHG emissions on a life cycle basis. The long-term dynamics of upstream processes are explored in this work to help guide future decarbonization policies.

Derived gaseous fuels

18/00112 Energy-efficient biogas reforming process to produce syngas: the enhanced methane conversion by O_2

Chen, X. *et al. Applied Energy*, 2017, 185, 687–697.

This study reports an energy-efficient biogas reforming process with high and stable methane conversions by O_2 presence. During this biogas reforming process, the effects of various O_2 concentrations in biogas on initial conversions and stability at various temperatures on a Ni/SiO_2 catalyst were detailed investigated. In addition, theoretical energy consumption and conversions were calculated based on the Gibbs energy minimization method to compare with experimental results. Carbon formation and sintering during the reforming process were characterized by thermal gravity analysis, the Brunauer–Emmett–Teller method, X-ray diffraction, and high-resolution transmission electron microscopy to investigate the feasibility of applying this process to an inexpensive nickel catalyst. The results showed that 5% O_2 in biogas improved the CH_4 conversion and stability of biogas reforming. The enhancement of stability was attributed to the inhibited sintering, the first finding, and the reduced carbon deposition at the same time, which sustained a stable conversion of CH_4, and proved the applicability of base Ni catalyst to this process. Higher O_2 concentrations ($\geq$10%) in biogas resulted in severe decrease in CO_2 conversion and greater H_2O productivity. The proposed biogas reforming process, with a high and stable conversion of CH_4, reduced energy input, and the applicability to inexpensive base metal catalyst, offers a good choice for biogas reforming with low O_2 concentrations ($\leq$5%) to produce syngas with high energy efficiency.

18/00113 Hydrocarbon gas generation from pyrolysis of extracts and residues of low maturity solid bitumens from the Sichuan Basin, China

Wang, Z. *et al. Organic Geochemistry*, 2017, 103, 51–62.

Two sets of pyrolysis experiments were performed on bitumen 'A' (BA) and extracted organic matter (ER) from low-maturity solid bitumen at heating rates of 2 and 20 °C/h in confined systems (gold capsules). The main observations can be listed as follows: (1) BA and ER have high generation potential of hydrocarbons and were a significant secondary hydrocarbon source. (2) Both have similar evolutionary characteristics of hydrocarbon gas generation, and have high C_1/C_{1-5} values than those from an Ordovician normal oil. E_a distributions of the methane generated from pyrolysis of BA and ER is far lower than that of Ordovician normal oil. (3) The evolution of stable carbon isotope values of individual hydrocarbon gases can be divided into three stages. Plots of $\ln C_1/C_2$ versus $\ln C_2/C_3$, $\delta^{13}C_1$–$\delta^{13}C_2$ versus $\ln(C_1/C_2)$ and $\delta^{13}C_2$–$\delta^{13}C_3$ versus $\ln(C_2/C_3)$ clearly illustrate the characteristics of hydrocarbon gases generated from BA and ER at different thermal maturity stages. (4) Basin modelling reconstructions of the hydrocarbon generation history of BA and ER in Sinian and Cambrian strata respectively indicate: Hydrocarbon gases generation from ER started in the Middle Jurassic, and ended in the Early Cretaceous with a maturity equivalent to Easy%Ro $\approx$ 2.2%. The final conversion rate of C_{1-5} and C_1 are 0.71 and 0.48, respectively. Hydrocarbon gas generation from BA started in the Early Jurassic, and ended in the Early Cretaceous with an Easy%Ro $\approx$ 3.0%. The final conversion rate of C_{1-5} and C_1 are 0.90 and 0.81, respectively.

18/00114 Mass and energy analysis of a 60 kW_{th} updraft gasifier using large size biomass

Ayyadurai, S. *et al. Fuel*, 2017, 187, 356–366.

An experimental study on an updraft gasifier (60 kW_{th}), using large size biomass as fuel, has been carried out to obtain the temperature profile, equivalence ratio, gas composition and its heating value. A theoretical mass and energy balance has allowed a proper justification of the experimental results obtained. The gasifier behaviour was studied in-depth using large size woody biomass to avoid the energy consumption required for chipping. The feedstock wood size was 1 m in length and

0.06 m in diameter and it was stacked 60 cm high, with a moisture content of 20%. Results were obtained for various flow conditions with air flow rates ranging from 20 to 30 m^3/h. Each test was carried out under continuous operation and steady state for 5 h. The different sub-processes taking place from top to bottom (grate) were under very transient conditions. Results for the temperature at the height of oxidation, reduction, pyrolysis and drying zones (23, 66, 78 and 92 cm, respectively) have been provided. The optimum gasifier behaviour was reached with an airflow rate of 20.66 m^3/h (or air inlet velocity of 1 m/s), leading to a producer gas heating value of 4500 kJ/N m^3 and a temperature of 955 °C at the oxidation stage. Comparison between the theoretical energy balance and thus derived from the tests have allowed for a better identification of the phenomena taking place during the particles conversion. Anyway, differences lower than 22% have been obtained in all the cases.

18/00115 Methane oxidation with low O_2/CH_4 ratios in the present of water: combustion or reforming

Geng, H. *et al. Energy Conversion and Management*, 2017, 132, 339–346.

This paper investigates the reaction of methane over copper and cobalt catalysts under oxygen-deficient conditions with added water. A fixed-bed reactor, TPD analysis, *in situ* DRIFTS study, and temperature detection were used to test the activity of the methane reaction, water adsorption on the metal surface, OH group behaviour, and the endothermic and exothermic processes of the reaction. The results show that the inhibitory effect of water mainly occurs at a low temperature and methane conversion decreases when water is introduced into the feed. Water easily adsorbs on metal clusters and forms OH groups at low temperatures. Copper tends to adsorb more water than cobalt and shows a stronger inhibitory effect. The DRIFTS spectra of the Cu catalyst show strong OH peaks during the reaction, of which the magnitudes increase with the water pressure. When the reaction temperature rises (750 °C), water begins to serve as an oxidant and participates in the reforming reaction. Both catalysts show a transition process between the oxidation and reforming reactions as the temperature increases. Co displays a better catalytic performance in the reforming reaction. Oxidation precedes reforming; water does not participate in the reaction if the oxygen is not fully consumed.

18/00116 Methane recovery from natural gas hydrate with simulated IGCC syngas

Ding, Y.-L. *et al. Energy*, 2017, 120, 192–198.

Methane (CH_4) recovery from natural gas hydrates (NGHs) by CO_2-CH_4 replacement is considered as a win-win technology for producing CH_4 and sequestrating CO_2 synchronously. In this investigation, simulated Integrated Gasification Combined Cycle (IGCC) syngas of CO_2/H_2 gas mixture is used to replace CH_4 from simulated methane hydrate which is formed in pure water at 274.15 K and 4.5 MPa. The changes of concentrations of CH_4, CO_2 and H_2 in gas phase during the replacement process are supervised by Gas Chromatograph (GC), and the gas hydrates are determined through *in situ* Raman. Meanwhile, the CH_4 recovery and the replacement mechanism are qualitatively analysed. The results indicate that, on one hand, the replacement consists of two steps, CH_4 hydrate dissociation at the first and followed by CO_2 hydrate formation, on the other hand, the CH_4 recovery from CH_4-CO_2/H_2 replacement is more than 71% which is significantly higher than that from CH_4-CO_2 replacement. Notably, no H_2 is found in the hydrate phase in the replacement process, which implying that H_2 does not compete with CH_4 molecules occupying hydrate cages but plays promotion role in CO_2–CH_4 replacement.

18/00117 Reaction of nitrous oxide with methane to synthesis gas: a thermodynamic and catalytic study

Khan, N. A. *et al. Journal of Energy Chemistry*, 2017, 26, (1), 155–162.

This study explores the coherence of thermodynamic equilibrium predictions with the actual catalytic reaction of CH_4 with N_2O, particularly at higher CH_4 conversions. For this purpose, key process variables, such as temperature (300–550 °C) and a molar feed ratio (N_2O/CH_4 = 1, 3 and 5), were altered to establish the conditions for maximized H_2 yield. The experimental study was conducted over the Co-ZSM-5 catalyst in a fixed bed tubular reactor and then compared with the thermodynamic equilibrium compositions, where the equilibrium composition was calculated via total Gibbs free energy minimization method. The results suggest that molar feed ratio plays an important role in the overall reaction products distribution. Generally for N_2O conversions, and irrespective of N_2O/CH_4 feed ratio, the thermodynamic predictions coincide with experimental data obtained at approximately 475–550 °C, indicating that the reactions are kinetically limited at lower range of temperatures. For example, theoretical calculations show that the H_2 yield is zero in presence of excess N_2O (N_2O/CH_4 = 5). However over a Co-ZSM-5 catalyst, and with a same molar feed ratio (N_2O/CH_4) of 5, the H_2 yield is initially 10% at 425 °C, while above 450 °C it drops to zero. Furthermore, H_2 yield steadily increases with temperature and with the level of CH_4 conversion for reactions limited by N_2O concentration in a reactant feed. The maximum attainable (from thermodynamic calculations and at a feed ratio of N_2O/CH_4 = 3) H_2 yield at 550 °C is 38%, whereas at same temperature and over Co-ZSM-5, the experimentally observed yield is about 19%. Carbon deposition on Co-ZSM-5 at lower temperatures and CH_4 conversion (less than 50%) was also observed. At higher temperatures and levels of CH_4 conversion (above 90%), the deposited carbon is suggested to react with N_2O to form CO_2.

18/00118 The effect of CO on coal–biomass co-gasification with CO_2

Farid, M. M. *et al. Fuel*, 2017, 188, 98–101.

In this study, co-gasification of coal and biomass chars with CO_2 in the presence of CO was investigated at three different temperatures: 850, 875 and 900 °C. A coal–biomass (bituminous–pineapple sawdust) mixture with a mass ratio of 1 : 1 was used for devolatilization and co-gasification. Random pore model was employed to determine the kinetic coefficient from experimentally obtained carbon conversion data. The Langmuir–Hinshelwood (L–H) equation, which has been widely used in literatures to describe the relationship between kinetic coefficient of the gasification and partial pressures of reacting gases, effectively represented the inhibition effect of CO on char–CO_2 gasification. The kinetic parameters of the L–H equation were acquired from the experimental data. The activation energy (E) and pre-exponential factor (A) of each kinetic parameter of L–H equation were obtained using the Arrhenius equation. CO inhibition effect was more powerful in the Char-CO_2 co-gasification of the mixed sample compared to those in the unmixed samples. Further, for each sample, the inhibition effect was stronger at lower temperature owing to a smaller number of active sites.

18/00119 Thermodynamic analyses for recovering residual heat of high-temperature basic oxygen gas (BOG) by the methane reforming with carbon dioxide reaction

Chen, L. *et al. Energy*, 2017, 118, 906–913.

For the recovery and utilization of high-temperature basic oxygen gas generated in the basic oxygen furnace process within iron and steel production, a thermochemical recovering method of tubular plug flow reaction is proposed. Accounting for efficient utilization of residual heat and capture of carbon dioxide, methane reforming with carbon dioxide reaction is introduced. With a linear-temperature heat source, the reacting rate, temperature and pressure distributions of mixed gas along the tubular reactor are obtained based on a thermodynamic model. The influences of three inlet parameters of temperature, total pressure, molar flow rate of methane, and a structure parameter of catalyst porosity are analysed. The results show that with the given conditions, the reacting rate firstly increases to the maximum and then decreases gradually nearly to zero, and the reforming reaction mainly occurs at the first half of the tube. The temperature increases with the flow along the tube, but the temperature gradient decreases on the contrary. The total pressure decreases and the pressure gradient gradually increases to a certain value at the end. Both of the inlet temperature and molar flow rate of methane have big influences on the reacting rate.

18/00120 Utilizing pyrolysis GC-MS to characterize organic matter quality in relation to methane production in a thermokarst lake sediment core

Heslop, J. *et al. Organic Geochemistry*, 2017, 103, 43–50.

Thermokarst (thaw) lakes are an important source of atmospheric CH_4; however, few studies have examined the composition and biodegradability of their sediment organic matter (OM). The authors have quantified the (i) composition of bulk sediment OM (bulk SOM) using pyrolysis gas chromatography-mass spectrometry (GC-MS) and (ii) statistical relationships between bulk SOM properties and anaerobic incubation CH_4 production rate at 3 °C in sediment core samples from a thermokarst lake system. The study extended through the full vertically-thawed profile (0–550 cm) of Vault Lake, a small thermokarst lake near Fairbanks, Alaska, USA, and into the permafrost thawing beneath the lake (551–590 cm). Compared with the underlying mineral-dominated sediments (153–590 cm depth in core), the surface organic-rich sediment horizon (0–152 cm) had higher CH_4 production rate, greater substrate availability indicated by percent organic carbon and total nitrogen, and greater proportions of terrestrially-associated bulk SOM compounds (alkanes, alkenes, lignin products, and phenols and phenolic precursors). Correlation and principal component analyses indicated that CH_4 production potential values measured in the core were positively associated with initial substrate availability and terrestrially-derived OM compounds. The authors observed positive correlation ($p \leq 0.05$) between CH_4 production and bulk SOM compounds classified as phenols and phenolic precursors, a pattern different from previously observed relationships in natural aquatic anaerobic environments.

18/00121 Water-gas shift reaction on alumina-supported Pt-CeO_x catalysts prepared by supercritical fluid deposition

Deal, J. W. *et al. The Journal of Supercritical Fluids*, 2017, 119, 113–121.

Alumina-supported platinum catalysts, both with and without ceria, were prepared by supercritical fluid deposition and evaluated for activity for water-gas shift reaction. The organometallic precursor, platinum(II) acetylacetonate, was deposited from solution in supercritical carbon dioxide. Analysis of the catalysts by high resolution scanning transmission electron microscopy indicated that platinum was present in the form of highly dispersed metal nanoparticles. Pretreatment of the alumina-supported ceria in hydrogen prior to the deposition of the platinum precursor resulted in more platinum nucleated on ceria than non-pretreated alumina-supported ceria but varied in both particle size and structure. The ceria-containing catalyst that was not pre-treated exhibited a more uniform particle size, and the Pt particles were encapsulated in crystalline ceria. Reaction rate measurements showed that the catalyst was more active for water-gas shift, with reaction rates per mass of platinum that exceeded most literature values for water-gas shift reaction on Pt-CeO_x catalysts. The high activity was attributed to the significant fraction of platinum/ceria interfacial contact. These results show the promise of supercritical fluid deposition as a scalable means of synthesizing highly active supported metal catalysts that offer efficient utilization of precious metals.

LNG

18/00122 A Monte Carlo approach to the ship-centric Markov decision process for analyzing decisions over converting a containership to LNG power

Kana, A. A. and Harrison, B. M. *Ocean Engineering*, 2017, 130, 40–48.

A Monte Carlo approach to the ship-centric Markov decision process (SC-MDP) is presented for analysing whether a container ship should convert to LNG power in the face of evolving emission control area regulations. The SC-MDP model was originally developed as a means to analyse uncertain, sequential decision making problems. However, the original model is limited in its handling of uncertainty by only using discrete probabilistic values to account for the uncertainty. This paper extends the model to include Monte Carlo simulations to gain a deeper understanding of how uncertainty affects decision-making behaviour. A case study is presented involving the impact of evolving emission control areas on the design and operation of a notional 13,000 TEU container ship. The decision of whether to invest in a dual fuel LNG engine is analysed given uncertainties in economic parameters, regulatory scenarios, and supply chain risks. The case study is used to show how variations in uncertain parameters can have a drastic effect on optimal decision strategies.

18/00123 A novel LNG/O_2 combustion gas and steam mixture cycle with energy storage and CO_2 capture

Chen, Y. *et al. Energy*, 2017, 120, 128–137.

A gas and steam mixture cycle (GSMC) is presented with a mixture of liquid natural gas/oxygen (LNG/O_2) combustion product and feedwater as working medium, integrating features of high efficiency power generation, peak shaving, energy storage and CO_2 capture. The liquefied oxygen is produced during off-peak hours. During the operation hours, the cryogenic liquids of both LNG and oxygen are pumped to a high pressure and preheated before entering the combustors through the burners. The combustion product heats and mixes with the atomized feedwater to form supercritical H_2O/CO_2 mixture vapour for power generation in a turbine unit. The CO_2 vapour is separated from condensate water in the condenser and liquefied by the cryogenic liquids of both LNG and oxygen after being compressed to a higher pressure. The circulation feedwater is injected to the annular channel between flame tube and shell cylinder of modular combustor via feedwater heating system. The results show that under the conditions of turbine inlet parameters of 40 MPa/800 °C and condensation temperature of 30 °C, the output power efficiency based on the thermal value of LNG fuel is 49.2% and the equivalent net efficiency is 46.4%, which accounts for one quarter of off-peak electricity consumption for liquid O_2 production.

18/00124 Multi-level explosion risk analysis (MLERA) for accidental gas explosion events in super-large FLNG facilities

Huang, Y. *et al. Journal of Loss Prevention in the Process Industries*, 2017, 45, 242–254.

When assessing explosion risks of super-large offshore structures such as floating liquefied natural gas (FLNG) facilities, there are neither design rules nor industry standards available as FLNG is a new technology. Meanwhile, a large amount of computational fluid dynamic (CFD) calculation time is required due to its super-large size and highly complicated topside structures. A multi-level explosion risk analysis method (MLERA) is developed in this paper, which divides the whole structure into subsections and applies detailed CFD calculations only to the areas with the highest level of potential risks so that the computational time can be reduced to a realistic and acceptable level. The MLERA includes three levels, which are qualitative risk screening, semi-quantitative risk classification, and quantitative risk assessment. A CFD tool called FLACS is used as a calculation tool for detailed risk quantification, and an ALARP (as low as reasonably practical) method is selected as a calibration tool and used to determine the acceptance of the explosion risk. Meanwhile, since the current design standards for normal offshore platforms are not sufficient for super-large structures, during the risk screening and risk classification processes, safety barriers are used as extra risk indicators in addition to the traditional ones. A case study is conducted based on a cylindrical FLNG model, and the result of the case study proves that the proposed MLERA method is able to save a large amount of computational time.

18/00125 Review of propulsion systems on LNG carriers

Fernández, I. A. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 1395–1411.

Vessel ozone depleting emission regulations are regulated in Annex VI of the MARPOL Convention, wherein the maximum levels of NO_x, SO_x and suspended particles are established. These increasingly strict regulations, together with the increase in natural gas consumption and its price, have conditioned propulsion systems implemented on board vessels. This article reviews the different propulsion systems used on board vessels for the transport of liquefied natural gas. The study describes the main characteristics of the propulsion systems, and the advantages and drawbacks that come along with these, from its very beginnings up to the systems installed to date. The described propulsion systems include both gas and steam turbines, combined cycles, two- and four-stroke internal combustion engines, as well as reliquefaction plants, while encompassing mechanical, electric and dual fuel (DF) technology systems. The propulsion systems implemented have undergone continual alteration in order to adjust to market needs, which were always governed by both efficiency and the possibility of consuming boil-off gas (BOG), always in compliance with the strict antipollution regulations in force. The current direction of LNG vessel propulsion systems is the installation of two-stroke DF low pressure engines due to their high efficiency and their possibility of installing a BOG reliquefaction plant. Another great advantage of this propulsion system is its compliance with the IMO TIER III emission regulations, without the need to install any supplementary gas treatment system.

Hydrogen generation and storage

18/00126 A comparative overview of hydrogen production processes

Nikolaidis, P. and Poullikkas, A. *Renewable and Sustainable Energy Reviews*, 2017, 67, 597–611.

Climate change and fossil fuel depletion are the main reasons leading to hydrogen technology. There are many processes for hydrogen production from both conventional and alternative energy resources such as natural gas, coal, nuclear, biomass, solar and wind. In this work, a comparative overview of the major hydrogen production methods is carried out. The process descriptions along with the technical and economic aspects of 14 different production methods are discussed. An overall comparison is carried out, and the results regarding both the conventional and renewable methods are presented. The thermochemical pyrolysis and gasification are economically viable approaches providing the highest potential to become competitive on a large scale in the near future while conventional methods retain their dominant role in H_2 production with costs in the range of 1.34–2.27 $/kg. Biological methods appear to be a promising pathway but further research studies are needed to improve their production rates, while the low conversion efficiencies in combination with the high investment costs are the key restrictions for water-splitting technologies to compete with conventional methods. However, further development of these technologies along with significant innovations concerning H_2 storage, transportation and utilization, implies the decrease of the national dependence on fossil fuel imports and green hydrogen will dominate over the traditional energy resources.

18/00127 A new solar receiver/reactor structure for hydrogen production

Wang, Y. *et al. Energy Conversion and Management*, 2017, 133, 118–126.

Energy level matching of provided solar thermal energy with the involved reaction is important in determining the performances of a receiver/reactor. According to the main idea, i.e. minimizing irreversibility between the collected solar energy and the required reaction heat can increase the solar-to-fuel energy conversion efficiency, in this study a new mid- and low-temperature solar receiver/reactor structure is proposed to match the concentrated solar energy level with the chemical reaction in a catalytic bed by changing the aperture width, diameter and length of the receiver/reactor tube along the flow direction. A multi-field coupling mathematical model that incorporates mass, fluid flow, energy conservation governing equations, and the kinetic model of the methanol steam reforming (MSR) is developed to investigate the performances of the new structure and the traditional structure. Results showed that the MCR increases by reducing the aperture width, meanwhile the maximum catalyst bed temperature (MCBT) can be reduced by 17.9 °C. The performance of the solar receiver/reactor can be further improved when the diameter and the aperture changes harmonious along the flow direction. The new structure exhibits 8.35–15.85% higher MCR than the traditional structure. As a result, a new insight is introduced for the design of the receiver/reactor structure.

18/00128 Heavy metal-free, near-infrared colloidal quantum dots for efficient photoelectrochemical hydrogen generation

Tong, X. *et al. Nano Energy*, 2017, 31, 441–449.

Photoelectrochemical (PEC) hydrogen generation based on colloidal quantum dots (QDs) is very promising because of its high solar energy to fuel conversion efficiency and low fabrication costs. However, its commercial development is hindered by various challenges, including the widespread use of toxic heavy metal-based QDs as sensitizers. This study reports an environmentally friendly, high efficiency PEC device in which the photoanode consists of a mesoporous TiO_2 film sensitized with heavy metal-free, near-infrared (NIR) colloidal $CuInSe_xS_{2-x}$ (CISeS) QDs. To reduce surface-related traps, the authors grew an ultrathin ZnS shell on the CISeS core QDs by cation exchange. The PEC cell based on this core/shell CISeS/ZnS QDs exhibits suppressed charge recombination and a saturated photocurrent density of $\sim$5.3 mA/cm^2 under one sun illumination (AM 1.5 G, 100 mW/cm^2). In addition, the as-prepared PEC device shows an outstanding stability, exhibiting a drop of only 23% after 9 h illumination. The success in using such core/shell CISeS/ZnS QDs paves the way to realize environment-friendly, high efficiency and cost-effective PEC devices for hydrogen production.

18/00129 In-situ investigation of the hydrogen release mechanism in bulk Mg_2NiH_4

Tran, X. Q. *et al. Journal of Power Sources*, 2017, 341, 130–138.

Hydrogen storage is an important aspect to enable the so-called hydrogen economy. Mg-Ni alloys are among the most promising candidates for solid-state hydrogen storage systems yet many questions remain unanswered regarding the hydriding/dehydriding mechanism of the alloys. Mg_2NiH_4 particularly has received much attention both for its potential as a hydrogen storage medium and also exhibits interesting properties relating to its different polymorphs. Here, the dehydriding mechanism in bulk Mg_2NiH_4 is investigated using *in situ* ultra-high voltage transmission electron microscopy (TEM) combined with synchrotron powder X-ray diffraction and differential scanning calorimetry (DSC). It was found that the hydrogen release is based on a mechanism of nucleation and growth of Mg_2NiH_x ($x \sim 0$–0.3) solid solution grains and is greatly enhanced in the presence of crystal defects occurring as a result of the polymorphic phase transformation. Also importantly, with atomic resolution TEM imaging a high density of stacking faults is identified in the dehydrided Mg_2NiH_x ($x \sim 0$–0.3) lattices.

18/00130 Metal-free pyridinium-based polymeric ionic liquids as catalyst for H_2 generation from $NaBH_4$

Sahiner, N. *et al. Renewable Energy*, 2017, 101, 1005–1012.

Monodispersed poly(2-vinyl pyridine) (p(2-VP)) polymeric particles were synthesized with a self-emulsion polymerization (SEP) technique. Polymeric ionic liquid (PIL) particles such as poly(2-vinyl pyridine)-ethane (p(2-VP)$^{++}C_2$), poly(2-vinyl pyridine)-butane (p(2-VP)$^{++}C_4$), and poly(2-vinyl pyridine)-hexane (p(2-VP)$^{++}C_6$) particles were then prepared from monodispersed p(2-VP) particles by modifying with 1,2-dibromobutane (DBE) 1,4-dibromobutane (DBB) and 1,6-dibromobutane (DBH), respectively. The hydrodynamic diameter of the prepared particles was found be in the range of 350–400 nm, and the zeta potential of p(2-VP)$^{++}C_n$ (n: 2, 4 and 6) particles were found to be in the range of 26–28 mV. The prepared PIL particles (p(2-VP)$^{++}C_6$, etc.) were shown to be very effective catalysts in H_2 generation by methanolysis of $NaBH_4$. Various parameters, such as the effect of modifying agents on PIL particle, the amount of PIL particles, the amount of $NaBH_4$ and temperature, affecting the H_2 production rate were investigated. Hydrogen generation rate (HGR) was calculated as 5433 ± 141 mL $H_2\,g^{-1}\,min^{-1}$ for 50 mg p(2-VP)$^{++}C_6$ particles in the methanolysis of 500 mM $NaBH_4$. The activation energy (Ea) of methanolysis of $NaBH_4$ catalysed by p(2-VP)$^{++}C_6$ particles was calculated as 20.84 ± 0.76 kJ mol^{-1}, which is much lower than similar studies reported in the literature.

18/00131 Photocatalytic activity of MAl_2O_4 (M = Mg, Sr and Ba) for hydrogen production

Gómez-Solís, C. *et al. Fuel*, 2017, 188, 197–204.

This work reports the hydrogen production of aluminate spinel type materials, MAl_2O_4 (M = Mg, Sr, and Ba), prepared by solid state method. Characterization was carried out by means of X-ray diffraction (XRD), scanning electronic microscopic (SEM), UV–vis spectroscopy, BET method, chronoamperometry, and EIS. Through electrochemical impedance and UV–vis spectroscopy it was possible the determination of the valence and conduction band edge potential, to define the transfer charge mechanism during the hydrogen production reaction. The photocatalytic measurements coupled with a gas chromatographic system indicated that $MgAl_2O_4$ showed the best rate of $7.3\,\mu mol \cdot g^{-1} \cdot h^{-1}$ for magnesium aluminate, without any co-catalyst or sacrificial reagent. The tendency of the photocatalytic activity for hydrogen production in this work is as follows: $MgAl_2O_4 > BaAl_2O_4 > SrAl_2O_4$. When Al_2O_3 was used as co-catalyst mixed with Magnesium aluminate ($MgAl_2O_4$), the photoactivity was enhanced, increasing up to nine times the hydrogen production (64 vs $7.3\,\mu mol \cdot g^{-1} \cdot h^{-1}$). Additionally, photo-corrosion test indicated that all samples were chemically stable under irradiation conditions.

18/00132 Single crystal $CsTaWO_6$ nanoparticles for photocatalytic hydrogen production

Weller, T. *et al. Nano Energy*, 2017, 31, 551–559.

Due to its band positions and unique crystal structure, $CsTaWO_6$ is a very interesting model system for the investigation of morphological influences on the performance in photocatalytic Hydrogen generation and water splitting. Here the authors present the synthesis of phase-pure and single crystal $CsTaWO_6$ nanoparticles in the range of 8–30 nm via hydrothermal synthesis. The nanoparticle size was controlled by adjusting the amount of base in the synthesis. Nanoparticles of different sizes were used to perform photocatalytic Hydrogen generation from water/methanol. The optimum particle size was found to be around 13 nm with regard to maximum gas evolution activity.

18/00133 Surface plasmon resonance enhancement of production of H_2 from ammonia borane solution with tunable $Cu_{2-x}S$ nanowires decorated by Pd nanoparticles

Liu, P.-H. *et al. Nano Energy*, 2017, 31, 57–63.

Localized surface plasmon resonances (LSPR) in near-infrared (NIR) region have been extensively studied for copper chalcogenide nanostructures, not only for the absorption enhancement but also tuneable LSPR characteristics with their free carrier concentrations or defects. In this study, a one-step cation exchange method has been used to synthesize $Cu_{2-x}S$ nanowires with x varying between 0 and 1, including Cu_2S, Cu_7S_4 and CuS and so forth. The plasmonic band of $Cu_{2-x}S$ nanowires shifts to a shorter wavelength with the increase in x, as observed in vis-NIR spectra, which is attributed to the increase in density of copper vacancies. The $Cu_{2-x}S$ nanowires have been used as catalysts towards the photocatalytic generation of H_2 from ammonia borane (AB). Among samples with different Cu–S compositions, Cu_7S_4 samples exhibited the highest activity in terms of H_2 evolution rate (25.54 mmol/g h). Moreover, a marked enhancement of the H_2 evolution rate (157.04 mmol/g h) could be achieved after decorating the $Cu_{2-x}S$ nanowires with Pd nanoparticles to form the hybrid structures. The results of this investigation may lead to an effective strategy for the design and development of LSPR materials for photocatalytic applications.

18/00134 Thermoeconomic modeling and optimization of a hydrogen production system using geothermal energy

Yilmaz, C. *Geothermics*, 2017, 65, 32–43.

Thermoeconomic optimization procedure is applied using genetic algorithm method to an integrated system composed of an alkaline water electrolysis unit for hydrogen production and a combined flash-binary geothermal power plant for providing power input to the electrolysis unit. The objective is to minimize the unit costs of the products (electricity and hydrogen production) of the composed system. The optimization approach is developed based on the cost optimal exergetic efficiency that is obtained for a component isolated from the remaining of the system components. Objectives to be optimized given certain constraints and variables are developed for each subcomponent of the system. Using genetic algorithm method of optimization, the variables, relative cost differences, and exergetic efficiencies with the corresponding optimal values are obtained. Thermoeconomic optimal values for product cost flow rate, fuel cost flow rate, unit cost of electricity, and unit cost of hydrogen production

are calculated to be 2412 $/h, 289.4 $/h, 0.01066 $/kWh, and 1.088 $/kg, respectively, whereas the corresponding actual base case values are 2607 $/h, 295.9 $/h, 0.01105 $/kWh, and 1.149 $/kg, respectively.

04 BY-PRODUCTS RELATED TO FUELS

18/00135 Autothermal reforming of heavy-hydrocarbon fuels by morphology controlled perovskite catalysts using carbon templates

Jeon, Y. *et al. Fuel*, 2017, 187, 446–456.

A novel synthesis of morphology-controlled perovskite networked with $LaCr_{0.8}Ru_{0.2}O_3$ nanoparticles was introduced using activated carbons as sacrificial templates. These catalysts were used for the hydrogen production by heavy-hydrocarbon autothermal reforming. To investigate the effect of the carbon templates, morphology-controlled perovskites using activated carbons and a non-templated catalyst were prepared to determine how carbon templates influence the chemical structure of the perovskite. The carbon templates produced a crystalline structure with the well incorporation of Ru under mild calcination conditions. The morphology of the hollow fibres provided a higher specific surface area than that of the porous grain catalyst with a similar average particle size (~80 nm). It was found that the hollow fibres showed a unique pore structure with large macropores from 1 to 100 μm, which might offer a higher surface area and enhanced mass transfer of the reactants. This provided a higher activation energy for H_2 production than the porous grain and non-templated catalysts during the autothermal reforming of heavy hydrocarbons. As a result, the fibrous feature and well-defined chemical structure were crucial factors when cracking the hydrocarbon chain. The hollow fibre catalyst showed high reforming efficiency for H_2 production (>65 mol%) from heavy-hydrocarbon fuels during long-term experiments, featuring substantial durability with low carbon deposition and no structural changes.

18/00136 Influence of the biomass components on the pore formation of activated carbon

Correa, C. R. *et al. Biomass and Bioenergy*, 2017, 97, 53–64.

Uncontrolled management of agricultural wastes has strongly contributed to the increase of greenhouse emissions and pollution. On the other hand, these residues can be used as a sustainable source for the production of activated carbon. Currently, biomasses rich in lignin are the most widely used, due to the high yields and large surface areas attainable. The aim of this study is to understand the influence of each biomass component on activated carbon properties. Alpha-cellulose, xylan, kraft lignin, and mixtures with different ratios of the single components were used as model substances to represent biomass. These materials were pyrolysed and subsequently activated with KOH to expand the surface area. TGA results showed no interaction between components during pyrolysis but there was a strong influence of the composition of the mixture on the activated carbon properties due to the different thermal stabilities of each char. The activated carbon with the largest apparent surface area was obtained from cellulose with 2220 $m^2 g^{-1}$ and pure xylan showed the lowest with 1950 $m^2 g^{-1}$. T-plot calculations showed that more than 90% of the surface area was composed by micropores. To understand the microporosity, CO_2 isotherms were measured. The surface areas calculated were lower but followed the same trend as those obtained from the isotherms with N_2.

18/00137 Kinetic studies of mercury adsorption in activated carbon modified by iodine steam vapor deposition method

Zhong, L. *et al. Fuel*, 2017, 188, 343–351.

The objective of this study was to develop a high efficiency activated carbon (AC) sorbent for mercury removal. The vapour deposition method was used to modify the raw AC. This method is relatively easy to carry out and uniformly modifies the AC. The results of this study indicate that AC modified by iodine steam vapour deposition has much better Hg capturing capacity than AC modified by bromide deposition under the same experimental conditions. London dispersion forces and exposure of the sorbent surfaces play important roles in elemental mercury (Hg^0) adsorption. Adsorption kinetic behaviour was also studied under different experiment conditions. Results indicated that the pseudo-second model was the best fit to the actual mercury adsorption behaviour onto AC-I_2 sorbent. The effect of adsorbent mass and gas flow rate on adsorption behaviour were examined. Results indicated that increasing the sorbent mass led to an increase in Hg adsorption capacity, while increasing the gas flow rate resulted in a significant decrease in Hg adsorption capacity. Decreases in Hg adsorption capacity were likely due to a shorter contact time and lower partial pressure reducing the number of contact opportunities between the Hg atoms and the sorbent surface. Finally, a general dynamic equation was determined that can be used to help predict Hg adsorption curve of AC-I_2 sorbent without completing a real fixed-bed Hg adsorption experiment.

18/00138 Leaching mechanisms of constituents from fly ash under the influence of humic acid

Zhao, S. *et al. Journal of Hazardous Materials*, 2017, 321, 647–660.

As a low-cost material for adsorption, FA is one of the most efficient adsorbents of HA. However, the leaching of elements from FA is problematic during utilization in water treatment. In this investigation, the potential leaching behaviours of calcium, arsenic, boron, chromium, and other elements from FA in HA solution were studied via batch test. The data show that HA had an effect on the leaching of each element of FA, depending on the pH, the initial concentration of HA and the addition of calcium oxide (CaO). The Langmuir isotherm could better fit the equilibrium data in different initial concentrations of HA from 10 to 100 mg/L. Because of the interaction between HA and the FA leaching elements, multi-layer adsorption occurred when the initial concentration of HA was more than 100 mg/L. The pH and free CaO content played major roles in HA adsorption and FA leaching. Using SEM and XRD to characterize the solid of FA being mixed with CaO treated in solution, the results demonstrated that the reaction between FA and CaO could generate crystal minerals, such as portlandite, gismondine, ettringite (AFt) and calcite, which effectively restrained the leaching of elements, reduced secondary pollution.

18/00139 Regeneration of sulfamethoxazole-saturated activated carbon using gamma irradiation

Chu, L. and Wang, J. *Radiation Physics and Chemistry*, 2017, 130, 391–396.

Activated carbon (AC) has been widely used for reclamation and reuse of the effluent of wastewater treatment plant to further remove the emerging contaminants, such as PPCPs in recent years. How to regenerate the exhausted AC effectively and economically is still a challenge. In the present study, the regeneration of AC exhausted with SMX was performed by gamma irradiation to simultaneously recover the spent AC and degrade the pollutants. The results showed that the adsorption of SMX onto AC can be described by the Langmuir isotherm and the adsorption capacity was about 417 mg/g. SMX can be removed rapidly when exposed to gamma irradiation, with the initial concentration of 100 mg/L, more than 99% of SMX was removed at 5.0 kGy, while an extremely high dose (150 kGy) was needed to reach 80% mineralization ratio. The regeneration efficiency was about 21–30% at 50–200 kGy. The absorbed SMX and the intermediates formed during gamma irradiation were released into aqueous solution from AC and mineralized, leading to the partial regeneration of the adsorption capacity of AC. Further studies are needed to optimize the experimental conditions to increase the regeneration efficiency.

18/00140 The influence of crystallization on the flow of coal ash-slags

Seebold, S. *et al. Fuel*, 2017, 187, 376–387.

Numerous technical applications in the energy and metallurgical industries demand a fundamental knowledge of the flow of slags. In particular, the operation of an entrained flow gasifier is challenging, as the oxide slag has to be reliably discharged. Crystallization in the slag influences strongly the flow behaviour of the slag because precipitations occur. In this study, the process of crystallization during flow of two coal ash slags was investigated. Therefore, isothermal viscosity measurements were conducted in order to examine the rheological evolution over time caused by the crystallization. It has been demonstrated that the evolution of viscosity of a sub-liquidus melt depends strongly on time, as well as on temperature and composition. Using a rotational high-temperature viscometer to investigate coal slags, it was found that the crystallization during flow could be separated into three time regimes: a lag-time, in which the undercooled melt behaved as an Arrhenius-liquid; the kinetic-driven crystallization; and, finally, the rheological equilibrium that is represented by a constant viscosity. Furthermore, an increase of relative viscosity caused by crystallization was accompanied by a shift from Newtonian to non-Newtonian flow; here, pseudoplastic flow indicated the existence of precipitations. The results demonstrate that the flow behaviour has to be divided into dilute, semi-concentrated and concentrated particle bearing fluids. A view into the morphology of the partly crystallized slag was taken by scanning electron microscope. Differential thermal analysis of the slags was conducted, to underline the results of the isothermal viscosity measurements. The degree of supercooling promotes the kinetics of crystallization. The results demonstrate that time-dependency has to be considered for an accurate description of flow during crystallization, as well as the influence of degree of supercooling.

18/00141 Toxicity assessment of carbon black waste: a by-product from oil refineries

Zhen, X. *et al. Journal of Hazardous Materials*, 2017, 321, 600–610.

In Singapore, approximately 30 t/day of carbon-based solid waste are produced from petrochemical processes. This carbon black waste has been shown to possess physical properties that are characteristic of a good adsorbent such as high external surface area. Therefore, there is a growing interest to reutilize and process this carbon black waste into secondary materials such as adsorbents. However, the carbon black waste obtained from petrochemical industries may contain heavy metals that are hazardous to human health and the environment, hence restricting its full potential for re-utilization. Therefore, it is important to examine the possible toxicity effects and toxicity mechanism of carbon black waste on human health. In this study, inductively coupled plasma optical emission spectroscopy (ICP-OES) analysis showed that the heavy metals, vanadium (V), molybdenum (Mo) and nickel (Ni), were present in the carbon black waste in high concentrations. Three human cell lines (HepG2 cells, MRC-5 cells and MDA-MB-231 cells) were used to investigate the toxicity of carbon black waste extract in a variety of in vitro assays. Results from MTS assays indicated that carbon black waste extract decreased the viability of all three cell lines in a dose and time-dependent manner. Observations from confocal microscopy further confirmed this phenomenon. Flow cytometry assay also showed that carbon black waste extract induced apoptosis of human cell lines, and the level of apoptosis increased with increasing waste concentration. Results from reactive oxygen species (ROS) assay indicated that carbon black waste extract induced oxidative stress by increasing intracellular ROS generation in these three human cell lines. Moreover, induction of oxidative damage in these cells was also observed through the alteration of glutathione (GSH) and superoxide dismutase (SOD) activities. Last but not least, by treating the cells with V-spiked solution of concentration equivalent to that found in the carbon black waste extract, V was identified as the main culprit for the high toxicity of carbon black waste extract. These findings could potentially provide insight into the hazards of carbon black waste extract and its toxicity mechanism on human cell lines.

05 NUCLEAR FUELS

Scientific, technical

18/00142 Large-scale large eddy simulation of nuclear reactor flows: issues and perspectives

Merzari, E. *et al. Nuclear Engineering and Design*, 2017, 312, 86–98.

Numerical simulation has been an intrinsic part of nuclear engineering research since its inception. In recent years a transition is occurring toward predictive, first-principle-based tools such as computational fluid dynamics. Even with the advent of petascale computing, however, such tools still have significant limitations. In the present work some of these issues, and in particular the presence of massive multiscale separation, are discussed, as well as some of the research conducted to mitigate them. Petascale simulations at high fidelity (large eddy simulation/direct numerical simulation) were conducted with the massively parallel spectral element code Nek5000 on a series of representative problems. These simulations shed light on the requirements of several types of simulation: (1) axial flow around fuel rods, with particular attention to wall effects; (2) natural convection in the primary vessel and (3) flow in a rod bundle in the presence of spacing devices. The focus of the work here is on the lessons learned and the requirements to perform these simulations at exascale. Additional physical insight gained from these simulations is also emphasized.

18/00143 A comparative assessment of the fracture toughness behavior of ferritic-martensitic steels and nanostructured ferritic alloys

Byun, T. S. *et al. Journal of Nuclear Materials*, 2017, 484, 157–167.

The Fe–Cr alloys with ultrafine microstructures are primary candidate materials for advanced nuclear reactor components because of their excellent high temperature strength and high resistance to radiation-induced damage such as embrittlement and swelling. Mainly two types of Fe–Cr alloys have been developed for the high temperature reactor applications: the quenched and tempered ferritic-martensitic (FM) steels hardened primarily by ultrafine laths and carbonitrides and the powder metallurgy-based nanostructured ferritic alloys (NFAs) by nanograin structure and nanoclusters. This study aims at elucidating the differences and similarities in the temperature and strength dependences of fracture toughness in the Fe–Cr alloys to provide a comparative assessment of their high-temperature structural performance. The K_{JO} versus yield stress plots confirmed that the fracture toughness was inversely proportional to yield strength. It was found, however, that the toughness data for some NFAs were outside the band of the integrated dataset at given strength level, which indicates either a significant improvement or deterioration in mechanical properties due to fundamental changes in deformation and fracture mechanisms. When compared to the behaviour of NFAs, the FM steels have shown much less strength dependence and formed narrow fracture toughness data bands at a significantly lower strength region. It appeared that at high temperatures $\geq$600 °C the NFAs cannot retain the nanostructure advantage of high strength and high toughness either by high-temperature embrittlement or by excessive loss of strength. Irradiation studies have revealed, however, that the NFAs have much stronger radiation resistance than tempered martensitic steels, such as lower radiation-induced swelling, finer helium bubble formation, lower irradiation creep rate and reduced low temperature embrittlement.

18/00144 A study on wear behaviour of Al/6101/graphite composites

Sharma, P. *et al. Journal of Asian Ceramic Societies*, 2017, 5, (1), 42–48.

The current research work scrutinizes aluminium alloy 6101-graphite composites for their mechanical and tribological behaviour in dry sliding environments. The orthodox liquid casting technique had been used for the manufacturing of composite materials and imperilled to T6 heat treatment. The content of reinforcement particles was taken as 0, 4, 8, 12 and 16 wt% of graphite to ascertain it is prospective as self-lubricating reinforcement in sliding wear environments. Hardness, tensile strength and flexural strength of cast Al6101 metal matrix and manufactured composites were evaluated. Hardness, tensile strength and flexural strength decreases with increasing volume fraction of graphite reinforcement as compared to cast Al6101 metal matrix. Wear tests were performed on pin on disc apparatus to assess the tribological behaviour of composites and to determine the optimum volume fraction of graphite for its minimum wear rate. Wear rate reduces with increase in graphite volume fraction and minimum wear rate was attained at 4 wt% graphite. The wear was found to decrease with increase in sliding distance. The average co-efficient of friction also reduces with graphite addition and its minimum value was found to be at 4 wt% graphite. The worn surfaces of wear specimens were studied through scanning electron microscopy. The occurrence of 4 wt% of graphite reinforcement in the composites can reveal loftier wear possessions as compared to cast Al6101 metal matrix.

18/00145 Characterization of metallic fuel for minor actinides transmutation in fast reactor

Capriotti, L. *et al. Progress in Nuclear Energy*, 2017, 94, 194–201.

The METAPHIX programme is a collaboration between the Central Research Institute of Electric Power Industry (CRIEPI, Japan) and the Joint Research Centre–Institute for Transuranium Elements (JRC-ITU) of the European Commission dedicated to investigate the safety and effectiveness of a closed nuclear fuel cycle based on minor actinides (MA: Np, Am, Cm) separation from spent fuel, incorporation in metal alloy fuel and transmutation in fast reactor. Nine Na-bonded experimental pins of metal alloy fuel were prepared at ITU and irradiated at the Phenix reactor (CEA, France) achieving 2.5 at.%, 7 at.% and 10 at.% burn-up. Four metal alloy compositions were irradiated: U-Pu-Zr used as fuel reference, U-Pu-Zr + 5 wt.% MA, U-Pu-Zr + 2 wt.% MA + 2 wt.% Rare Earths (RE: Nd, Y, Ce, Gd), and +5 wt.% MA + 5 wt.% RE, respectively. RE reproduce the expected output of a pyrometallurgical reprocessing facility. Post-irradiation examination is performed using several techniques, covering properties ranging from the macroscopic morphology of the fuel matrix to the microanalysis of phases and elemental redistribution/segregation. The irradiated fuel is characterized by many phases occurring along the fuel radius. The fuel underwent large redistribution of the fuel constituents (U, Pu, Zr) and many secondary phases are present with a variety of compositions. The distribution of phases in the irradiated fuel containing minor actinides and rare earths is essentially similar to that observed in the basic ternary alloy fuel.

18/00146 Comparison of polyethersulfone and polyamide nanofiltration membranes for uranium removal from aqueous solution

Torkabad, M. G. *et al. Progress in Nuclear Energy*, 2017, 94, 93–100.

Dead-end filtration equipment was operated to evaluate the performance of polyethersulfone (PES-2) and polyamide (NF-1 and NF-2) membranes in terms of rejection and permeate flux for treatment of high-concentration uranium solutions under a variety of operational conditions. The optimum pH for uranium rejection using PES-2 was determined as 6 while the rejection increased significantly in polyamide membranes with increase of pH. The permeate flux of all membranes increased as the pressure increased from 5 to 20 bar while the uranium rejection by these membranes changed differently. As the feed

concentration increased from 7.5 to 238 mg/l, the uranium rejection by PES-2 decreased. On the contrary, the rejection by NF-1 and NF-2 increased from 57% to 79% and 62% to 98%, respectively. Also, the permeate flux of PES-2 was relatively constant whereas the permeate flux of polyamide membranes declined due to a decrease in the effective membrane pore size and an increase in osmotic pressure. The results showed that the nanofiltration process can be effectively employed for uranium removal from aqueous solutions.

18/00147 Detoxification and immobilization of chromite ore processing residue in spinel-based glass-ceramic

Liao, C.-Z. *et al. Journal of Hazardous Materials*, 2017, 321, 449–455.
A promising strategy for the detoxification and immobilization of chromite ore processing residue (COPR) in a spinel-based glass-ceramic matrix is reported in this study. In the search for a more chemically durable matrix for COPR, the most critical crystalline phase for Cr immobilization was found to be a spinel solid solution with a chemical composition of $MgCr_{1.32}Fe_{0.19}Al_{0.49}O_4$. Using Rietveld quantitative X-ray diffraction analysis, the authors identified this final product with the phases of spinel (3.5 wt%), diopside (5.2 wt%), and some amorphous contents (91.2 wt%). The partitioning ratio of Cr reveals that about 77% of the Cr was incorporated into the more chemically durable spinel phase. The results of Cr *K*-edge X-ray absorption near-edge spectroscopy show that no Cr(VI) was observed after conversion of COPR into a glass-ceramic, which indicates successful detoxification of Cr(VI) into Cr(III) in the COPR-incorporated glass-ceramic. The leaching performances of Cr_2O_3 and COPR-incorporated glass-ceramic were compared with a prolonged acid-leaching test, and the results demonstrate the superiority of the COPR-incorporated glass-ceramic matrix in the immobilization of Cr. The overall results suggest that the use of affordable additives has potential in more reliably immobilizing COPR with a spinel-based glass-ceramic for safer disposal of this hazardous waste.

18/00148 Effects of fuel relocation on reflood in a partially-blocked rod bundle

Kim, B. J. *et al. Nuclear Engineering and Design*, 2017, 312, 239–247.
Ballooning of the fuel rods has been an important issue, since it can influence the coolability of the rod bundle in a large-break loss-of-coolant accident (LBLOCA). Numerous past studies have investigated the effect of blockage geometry on the heat transfer in a partially blocked rod bundle. However, they did not consider the occurrence of fuel relocation and the corresponding effect on two-phase heat transfer. Some fragmented fuel particles located above the ballooned region may drop into the enlarged volume of the balloon. Accordingly, the fuel relocation brings in a local power increase in the ballooned region. The present study's objective is to investigate the effect of the fuel relocation on the reflood under a LBLOCA condition. Toward this end, experiments were performed in a 5×5 partially-blocked rod bundle. Two power profiles were tested: one is a typical cosine shape and the other is the modified shape considering the effect of the fuel relocation. For a typical power shape, the peak temperature in the ballooned rods was lower than that in the intact rods. On the other hand, for the modified power shape, the peak temperature in the ballooned rods was higher than that in the intact rods. Numerical simulations were also performed using the MARS code. The tendencies of the peak clad temperatures were well predicted.

18/00149 Erosion yield and W surface enrichment of Fe-W model system exposed to low flux deuterium plasma in the linear device GyM

Caniello, R. *et al. Nuclear Materials and Energy*, 2017, 10, 9–16.
Iron–tungsten (Fe–W) mixed films were exposed to the low flux deuterium plasma of GyM in order to study the behaviour of the sputtering yield with the ion fluence and temperature of the samples. From literature, it is known that an increase of the former lowers the Fe–W layers' sputtering yield as a consequence of the preferential sputtering of Fe leading to an enrichment in W of the outermost layers. An opposite trend was instead found for the latter probably due to the inter-diffusion of Fe and W (effective from 200 °C) resulting in the suppression of the W enrichment. Moreover, from 500 °C, also W segregation to the surface occurs. What is missing from literature is a systematic investigation of the role of temperature on W enrichment. In this work, dedicated experiments in GyM were carried out to fill this gap. After exposure, W enrichment was evaluated by Rutherford backscattering spectrometry (RBS) and inferred from measuring the eroded thickness of the samples using RBS and profilometer. Concerning the Fe–W sputtering yield as a function of fluence, it decreases by a factor of ~3 between the lowest ($3.0 \times 10^{22} D^+ m^{-2}$) and the highest fluence ($9.0 \times 10^{23} D^+ m^{-2}$) values considered. The other main result is that, at the lowest fluence, the exposure at room temperature leads to an erosion of the Fe–W samples more pronounced than that associated to the exposure at 500 °C.

18/00150 Instant release of fission products in leaching experiments with high burn-up nuclear fuels in the framework of the Euratom project FIRST-Nuclides

Lemmens, K. *et al. Journal of Nuclear Materials*, 2017, 484, 307–323.
The instant release of fission products from high burn-up UO_2 fuels and one MOX fuel was investigated by means of leach tests. The samples covered PWR and BWR fuels at average rod burn-up in the range of 45–63 GWd/t_{HM} and included clad fuel segments, fuel segments with opened cladding, fuel fragments and fuel powder. The tests were performed with sodium chloride–bicarbonate solutions under oxidizing conditions and, for one test, in reducing Ar/H_2 atmosphere. The iodine and cesium release could be partially explained by the differences in sample preparation, leading to different sizes and properties of the exposed surface areas. Iodine and cesium releases tend to correlate with FGR and linear power rating, but the scatter of the data is significant. Although the gap between the fuel and the cladding was closed in some high burn-up samples, fissures still provide possible preferential transport pathways.

18/00151 Magnetic graphene based nanocomposite for uranium scavenging

El-Maghrabi, H. H. *et al. Journal of Hazardous Materials*, 2017, 322, 370–379.
Magnetic graphene based ferberite nanocomposite was tailored by simple, green, low cost and industrial effective method. The microstructure and morphology of the designed nanomaterials were examined via XRD, Raman, FTIR, TEM, EDX and VSM. The prepared nanocomposites were introduced as a novel adsorbent for uranium ions scavenging from aqueous solution. Different operating conditions of time, pH, initial uranium concentration, adsorbent amount and temperature were investigated. The experimental data shows a promising adsorption capacity. In particular, a maximum value of 455 mg/g was obtained within 60 min at room temperature with adsorption efficiency of 90.5%. The kinetics and isotherms adsorption data were fitted with the pseudo-second order model and Langmuir equation, respectively. Finally, the designed nanocomposites were found to have a great degree of sustainability (above five times of profiteering) with a complete maintenance of their parental morphology and adsorption capacity.

18/00152 Neutron transmission and capture measurements and analysis of Dy from 0.01 to 550 eV

Block, R. C. *et al. Progress in Nuclear Energy*, 2017, 94, 126–132.
Neutron capture and transmission measurements were carried out from 0.01 to over 600 eV on both natural dysprosium (Dy) and samples highly enriched in ^{164}Dy. These data were analysed for resonance parameters utilizing the SAMMY Bayesian analysis code to simultaneously fit both the capture and transmission data. Parameters were obtained for 17 resonances in Dy isotopes up to 18 eV and for the ^{164}Dy resonances near 147, 450 and 540 eV. The thermal capture cross section (at 0.0253 eV) and capture resonance integral were determined for ^{164}Dy.

18/00153 Optimization of plutonium and minor actinide transmutation in an AP1000 fuel assembly via a genetic search algorithm

Washington, J. and King, J. *Nuclear Engineering and Design*, 2017, 311, 199–212.
The average nuclear power plant produces twenty metric tons of used nuclear fuel per year, which contains approximately 95 wt% uranium, 1 wt% plutonium, and 4 wt% fission products and transuranic elements. Fast reactors are the preferred option for the transmutation of plutonium and minor actinides; however, an optimistic deployment time of at least 20 years indicates a need for a near-term solution. Previous simulation work demonstrated the potential to transmute transuranic elements in a modified light water reactor fuel pin. This study optimizes a quarter-assembly containing target fuels coated with spectral shift absorbers for the transmutation of plutonium and minor actinides in light water reactors. The spectral shift absorber coating on the target fuel pin tunes the neutron energy spectrum experienced by the target fuel. A coupled model developed using the NEWT module from SCALE 6.1 and a genetic algorithm module from the DAKOTA optimization toolbox provided performance data for the burnup of the target fuel pins in this study. The optimization with the coupled NEWT/DAKOTA model proceeded in three stages. The first stage optimized a single-target fuel pin per quarter-assembly adjacent to the central instrumentation channel. The second stage evaluated a variety of quarter-assemblies with multiple target fuel pins from the first stage and the third stage re-optimized the pins in the optimal second stage quarter-assembly. An 8 wt% $PuZrO_2MgO$ inert matrix fuel pin with a 1.44 mm radius and a 0.06 mm Lu_2O_3 coating in a five target fuel pin per quarter-assembly configuration represents the optimal combination for the transmutation of plutonium and minor actinides in the LWR environment considered in this study.

18/00154 Probabilistic finite element investigation of prestressing loss in nuclear containment wall segments

Balomenos, G. P. and Pandey, M. D. *Nuclear Engineering and Design*, 2017, 311, 50–59.

The main function of the concrete containment structures is to prevent radioactive leakage to the environment in case of a loss of coolant accident (LOCA). The Canadian Standard CSA N287.6 (2011) proposes periodic inspections, i.e. pressure testing, in order to assess the strength and design criteria of the containment (proof test) and the leak tightness of the containment boundary (leakage rate test). During these tests, the concrete strains are measured and are expected to have a distribution due to several uncertainties. Therefore, this study aims to propose a probabilistic finite element analysis framework. Then, investigates the relationship between the concrete strains and the pre-stressing loss, in order to examine the possibility of estimating the average pre-stressing loss during pressure testing inspections. The results indicate that the concrete strain measurements during the leakage rate test may provide information with respect to the pre-stressing loss of the bonded system. In addition, the demonstrated framework can be further used for the probabilistic finite element analysis of real scale containments.

18/00155 Risk assessment of uranium hexafluoride release from a uranium conversion facility by using a fuzzy approach

Mohsendokht, M. *Journal of Loss Prevention in the Process Industries*, 2017, 45, 217–228.

Among industrial hazards, the release of toxic materials is of great importance to risk assessment of chemical industries. Uranium hexafluoride (UF_6) under some circumstances could be a very dangerous material to human health and the environment and in the case of release may have catastrophic consequences. In this study, the probability of UF_6 release from a uranium conversion facility was analysed by utilization of fault tree analysis (FTA) method. FTA is a well-known established technique in risk analysis of potential hazards. However, some shortcomings such as lack of reliability data are always a matter of concern in FTA application. To overcome this issue, expert elicitation and fuzzy set theory was applied. Results of the study showed the probability of 5.378×10^{-4} for UF_6 gas release from the uranium conversion systems. Importance and sensitivity analyses have also been conducted to evaluate the percentage contribution of each component to the top event occurrence and to identify the weak points of the whole facility. Through the study, it was determined that the operator failure and lack of a reliable automatic shut-down system are the two main important reasons for UF_6 release.

18/00156 The effect of fission-energy Xe ion irradiation on the structural integrity and dissolution of the CeO_2 matrix

Popel, A. J. *et al. Journal of Nuclear Materials*, 2017, 484, 332–338.

This work considers the effect of fission fragment damage on the structural integrity and dissolution of the CeO_2 matrix in water, as a simulant for the UO_2 matrix of spent nuclear fuel. For this purpose, thin films of CeO_2 on Si substrates were produced and irradiated by 92 MeV $^{129}Xe^{23+}$ ions to a fluence of 4.8×10^{15} ions/cm^2 to simulate fission damage that occurs within nuclear fuels along with bulk CeO_2 samples. The irradiated and unirradiated samples were characterized and a static batch dissolution experiment was conducted to study the effect of the induced irradiation damage on dissolution of the CeO_2 matrix. Complex restructuring took place in the irradiated films and the irradiated samples showed an increase in the amount of dissolved cerium, as compared to the corresponding unirradiated samples. Secondary phases were also observed on the surface of the irradiated CeO_2 films after the dissolution experiment.

18/00157 The investigation of vermiculite as an alternating shielding material for gamma rays

Gülbiçim, H. *et al. Radiation Physics and Chemistry*, 2017, 130, 112–117.

In this study, gamma ray shielding properties of vermiculite has been investigated for the first time as a shielding material. The photon total mass attenuation coefficients μ_m, the half value layer (HVL), the tenth value layer (TVL) and the mean free path (MFP) values have been experimentally determined for the photon energies at 0.244, 0.262, 0.342, 0.600, 0.778, 1.173, 1.332, 1.408 and 1.728 MeV. The theoretical data are calculated by using WinXCom computer code. At the end, good agreement was obtained between experimental and theoretical values. As well as the total mass attenuation coefficients, the authors have also calculated the effective atomic number, Z_{eff}, the effective electron number, N_{eff}, the total atomic cross-section, $\Sigma_{t,a}$, the total electronic cross-section, $\Sigma_{t,e}$, values for vermiculite and some building materials. Consequently, the obtained results showed that vermiculite could be used as a shielding material for gamma radiation.

18/00158 The MARINE experiment: irradiation of sphere-pac fuel and pellets of UO_{2-x} for americium breading blanket concept

D'Agata, E. *et al. Nuclear Engineering and Design*, 2017, 311, 131–141.

Americium is a strong contributor to the long-term radiotoxicity of high activity nuclear waste. Transmutation by irradiation in nuclear reactors of long-lived nuclides like ^{241}Am is therefore an option for the reduction of radiotoxicity and heat production of waste packages to be stored in a repository. The MARINE irradiation experiment is the latest of a series of European experiments on americium transmutation (e.g. EFTTRA-T4, EFTTRA-T4bis, HELIOS, MARIOS, SPHERE) performed in the high flux reactor (HFR). The MARINE experiment is developed and carried out in the framework of the collaborative research project PELGRIMM of the EURATOM Seventh Framework Programme (FP7). During the past years of experimental works in the field of transmutation and tests of innovative nuclear fuels, the release or trapping of helium as well as swelling have been shown to be the key issues for the design of such kind of fuel both as drivers and even more for Am-bearing blanket targets (due to the higher Am contents). The main objective of the MARINE experiment is to study the in-pile behaviour of uranium oxide fuel containing 13% of americium and to compare the behaviour of sphere-pac versus pellet fuel, in particular the role of microstructure and temperature on fission gas release and He on fuel swelling. The MARINE experiment will be irradiated in 2016 in the HFR in Petten (the Netherlands) and is expected to be completed in spring 2017. This paper discusses the rationale and objective of the MARINE experiment and provides a general description of its design for which some innovative features have been adopted.

18/00159 Tracking of fuel particles after pin failure in nominal, loss-of-flow and shutdown conditions in the MYRRHA reactor

Buckingham, S. *et al. Nuclear Engineering and Design*, 2017, 312, 137–146.

This work on fuel dispersion aims at quantifying the design and safety of the MYRRHA nuclear reactor. A number of accidents leading to the release of a secondary phase into the primary coolant loop are investigated. Among these scenarios, an incident leading to the failure of one or more of the fuel pins is simulated while the reactor is operating in nominal conditions, but also in natural convection regime either during accident transients such as loss-of-flow or during the normal shut-down of the reactor. Two single-phase CFD models of the MYRRHA reactor are constructed in ANSYS Fluent to represent the reactor in nominal and natural convection conditions. An Euler–Lagrange approach with one-way coupling is used for the flow and particle tracking. Firstly, a steady state RANS solution is obtained for each of the three conditions. Secondly, the particles are released downstream from the core outlet and particle distributions are provided over the coolant circuit. Their size and density are defined such that test cases represent potential extremes that may occur. Analysis of the results highlights different particle behaviours, depending essentially on gravity forces and kinematic effects. Statistical distributions highlight potential accumulation regions that may form at the free-surfaces, on top of the upper diaphragm plate or at the bottom of the vessel. These results help to localize regions of fuel accumulation in order to provide insight for development of strategies for accident mitigation.

18/00160 Tungsten oxide thin film exposed to low energy He plasma: evidence for a thermal enhancement of the erosion yield

Hijazi, H. *et al. Journal of Nuclear Materials*, 2017, 484, 91–97.

Nanocrystalline tungsten oxide thin films (about 75 nm in thickness) produced by thermal oxidation of tungsten substrates were exposed to low energy He plasma (≈20 eV/He) with a flux of 2.5×10^{18} m^{-2} s^{-1} at two temperatures: room temperature and 673 K. The structure and morphology modifications which occur after this He bombardment and annealing treatments was studied using Raman spectroscopy and transmission electron microscopy. Due to the low fluence (4×10^{21} m^{-2}) and low ion energy, few morphology modifications were observed after He plasma exposure at room temperature. On the contrary, at 673 K, a change in the layer colour was observed associated to an important erosion. Detailed analyses before/after exposure and before/after annealing allowed the authors to describe the He interaction with the oxide layer, its erosion and structural modification at the atomic and micrometre scale.

Economics, policy, supplies, forecasts

18/00161 Advances in multi-unit nuclear power plant probabilistic risk assessment

Modarres, M. *et al. Reliability Engineering & System Safety*, 2017, 157, 87–100.

The Fukushima Dai-ichi nuclear accident highlighted the importance of risks from multiple nuclear reactor unit accidents at a site. As a result, there has been considerable interest in multi-unit probabilistic risk assessment (MUPRA) in the past few years. For considerations in nuclear safety, the MUPRA estimates measures of risk and identifies contributors to risk representing the entire site rather than the individual units in the site. In doing so, possible unit-to-unit interactions and dependencies should be modelled and accounted for in the MUPRA. In order to effectively account for these risks, six main commonality classifications – initiating events, shared connections, identical components, proximity dependencies, human dependencies, and organizational dependencies – may be used. This paper examines advances in MUPRA, offers formal definitions of multi-unit site risk measures and proposes quantitative approaches and data to account for unit-to-unit dependencies. Finally, a parametric approach for the multi-unit dependencies has been discussed and a simple example illustrates application of the proposed methodology.

18/00162 CFD and experimental investigation of sloshing parameters for the safety assessment of HLM reactors

Myrillas, K. *et al. Nuclear Engineering and Design*, 2017, 312, 317–326.

For the safety assessment of heavy liquid metal nuclear reactors under seismic excitation, sloshing phenomena can be of great concern. The earthquake motions are transferred to the liquid coolant which oscillates inside the vessel, exerting additional forces on the walls and internal structures. The present study examines the case of MYRRHA, a multi-purpose experimental reactor with LBE as coolant, developed by SCK·CEN. The sloshing behaviour of liquid metals is studied through a comparison between mercury and water in a cylindrical tank. Experimental investigation of sloshing is carried out using optical techniques with the shaking table facility SHAKESPEARE at the von Karman Institute. Emphasis is given on the resonance case, where maximum forces occur on the tank walls. The experimental cases are reproduced numerically with the computational fluid dynamics (CFD) software OpenFOAM, using the VOF method to track the liquid interface. The non-linear nature of sloshing is observed through visualization, where swirling is shown in the resonance case. The complex behaviour is well reproduced by the CFD simulations, providing good qualitative validation of the numerical tools. A quantitative comparison of the maximum liquid elevation inside the tank shows higher values for the liquid metal than for water. Some discrepancies are revealed in CFD results and the differences are quantified. From simulations it is verified that the forces scale with the density ratio, following similar evolution in time. Overall, water is demonstrated to be a valid option as a working liquid in order to evaluate the sloshing effects, for forcing frequencies up to resonance.

18/00163 Earthquake-induced crustal deformation and consequences for fault displacement hazard analysis of nuclear power plants

Gürpinar, A. *et al. Nuclear Engineering and Design*, 2017, 311, 69–85.

Readily available interferometric data (InSAR) of the coseismic deformation field caused by recent seismic events clearly show that major earthquakes produce crustal deformation over wide areas, possibly resulting in significant stress loading/unloading of the crust. Such stress must be considered in the evaluation of seismic hazards of nuclear power plants (NPP) and, in particular, for the potential of surface slip (i.e. probabilistic fault displacement hazard analysis – PFDHA) on both primary and distributed faults. In this study, based on the assumption that slip on pre-existing structures can represent the elastic response of compliant fault zones to the permanent co-seismic stress changes induced by other major seismogenic structures, the authors propose a three-step procedure to address fault displacement issues and consider possible influence of surface faulting/deformation on vibratory ground motion (VGM). This approach includes: (a) data on the presence and characteristics of capable faults, (b) data on recognized and/or modelled co-seismic deformation fields and, where possible, (c) static stress transfer between source and receiving faults of unknown capability. The initial step involves the recognition of the major seismogenic structures nearest to the site and their characterization in terms of maximum expected earthquake and the time frame to be considered for determining their 'capability' (as defined in the International Atomic Energy Agency – IAEA Specific Safety Guide SSG-9). Then a GIS-based buffer approach is applied to identify all the faults near the NPP, possibly influenced by the crustal deformation induced by the major seismogenic structures. Faults inside these areas have to be tested for 'capability' according to the same time window defined for the primary seismogenic structures. If fault capability is confirmed or, eventually, cannot be assessed, the next step is to implement an approach based on the potential to affect the safety of the NPP site in terms of fault geometry, and potential displacement. Finally, in the case where the fault can affect the safety of the site, the third step is the PFDHA or, in other words, the calculation of the annual probability of exceedance of the potential co-seismic fault displacement; this displacement is to be compared with the fault displacement threshold that will impact the safety of the NPP site. The effect of site vicinity tectonism on site vibratory ground motion is also considered and an example in the light of the use of the ground motion prediction equations discussed.

18/00164 Estimation and comparison of the radionuclide inventories in vitrified high-level wastes from reprocessing plant

Caruso, S. *et al. Progress in Nuclear Energy*, 2017, 94, 216–221.

An accurate estimation of the radionuclide inventory of vitrified high-level waste is a prerequisite to assessing the radiological consequences of its geological disposal. The inventories of 34 radionuclides in this waste are provided by the waste producer for individual canisters at the time of loading/delivery. Of these, the inventories of 25 nuclides are measured directly during vitrification and the others are determined by calculation and/or correlation to measured contents. One purpose of the present work was to cross-check between the average and maximum radionuclide inventories of vitrified waste produced at the same facility in La Hague for Switzerland and Germany as of the data sets reported by the producer for 364 and 3017 canisters, respectively. Long-term safety assessments of geological repositories require the average and maximum inventories of a further 23 nuclides in addition to the 34 reported ones, which should be estimated by calculation or some correlation based on the technical specifications of the waste and of the reprocessing and vitrification processes. Another purpose of this work was therefore to cross-check these inventories and methods for their estimation as used by NAGRA and GRS. The results of this comparison show a good agreement for nuclides provided by the waste producer. The long-term safety relevant fission products show an agreement within 8%. The actinides have been found to show an agreement within 19%. The comparison between nuclides estimated on the basis of technical specifications shows higher deviations. The reasons for these discrepancies are addressed here.

18/00165 Numerical simulations of a mixed momentum-driven and buoyancy-driven jet in a large enclosure for nuclear reactor severe accident analysis

Carasik, L. B. *et al. Nuclear Engineering and Design*, 2017, 312, 161–171.

An ability to predict the behaviour of buoyant jets entering a large body of relatively stationary fluid is important in analysis of a wide variety of nuclear accidents, including for example the use of large tanks of water as heat sinks, or the release of hot gases into the secondary containment. In particular, the degree to which temperature stratification occurs is important, as it can affect markedly the effectiveness of the body of fluid as a heat sink. This paper reports the results of measurements on an experimental facility designed to exhibit such behaviour, and the results of attempts to predict this experiment using CFD. In particular, the authors investigate here the effectiveness of three alternative turbulence models for this analysis; low-Re k–ε, elliptic-blended k–ε and shear stress transport k–ω models. Both the degree of thermal stratification and the stability of the jet that were predicted differed markedly between the three models. Two of the models, the low-Re k–ε and the shear stress transport k–ω, tend to predict, wrongly, significant turbulent intensity in regions where fluid velocities are essentially zero. This spurious high turbulent intensity in turn causes (i) a high turbulent viscosity to be applied, wrongly stabilizing the jet and (ii) increased turbulent diffusion of heat, causing too deep and diffuse a stratification to be predicted.

18/00166 Probabilistic risk assessment of aircraft impact on a spent nuclear fuel dry storage

Almomani, B. *et al. Nuclear Engineering and Design*, 2017, 311, 104–119.

This paper proposes a systematic risk evaluation framework for one of the most significant impact events on an interim dry storage facility, an aircraft crash, by using a probabilistic approach. A realistic case study that includes a specific cask model and selected impact conditions is performed to demonstrate the practical applicability of the proposed framework. An event tree analysis of an occurred aircraft crash that defines a set of impact conditions and storage cask response is constructed. The Monte-Carlo simulation is employed for the probabilistic approach in consideration of sources of uncertainty associated with the impact loads onto the internal storage casks. The parameters for representing uncertainties that are managed probabilistically include the aircraft impact velocity, the compressive strength of the reinforced concrete wall, the missile shape factor, and the facility wall

thickness. Failure probabilities of the impacted wall and a single storage cask under direct mechanical impact load caused by the aircraft crash are estimated. A finite element analysis is applied to simulate the postulated direct engine impact load onto the cask body, and a source term analysis for associated releases of radioactive materials as well as an off-site consequence analysis are performed. Finally, conditional risk contribution calculations are represented by an event tree model. Case study results indicate that no severe risk is presented, as the radiological consequences do not exceed regulatory exposure limits to the public. This risk model can be used with any other representative detailed parameters and reference design concepts for other comparable direct or indirect impact conditions onto the cask body, which may provide an efficient way to investigate storage facility capacity to withstand an aircraft crash and thereby protect public health.

18/00167 Proposal for effective disposal options of very low level decommissioning waste

Choi, Y.-J. *et al. Progress in Nuclear Energy*, 2017, 94, 36–45.

The safe decommissioning of nuclear power plants is one of the key issues in Korea due to the aging of NPPs. In this paper effective disposal options to dispose very low level decommissioning waste have been described through analysis of the silo for radioactive waste in several countries including Korea, specifically focused on disposal of the large component waste and other very low level waste generated from NPP decommissioning. As a result of the analysis, compact silo farm is proposed with two options: those are (1) $\varnothing$ 22 × 23 m silo and (2) $\varnothing$ 8.6 × 22 m silo. Each option has two disposal methods; one-piece disposal and disposal after volume reduction are considered as disposal method. Furthermore, arrangement of large component and the shape of silo are also proposed in this study. Only steam generator is considered to be disposed of as a large component because it can be categorized as very low level waste. In terms of disposal arrangement of steam generator, there are two ways: one-by-one disposal and disposal in pairs. To decrease the size of silo, both cylindrical and rectangular shapes are considered. In addition, the required number of silos and capacity are also estimated so that a comparison can be made between two options.

18/00168 Radioactive contamination of several materials following the Fukushima Daiichi Nuclear Power Station accident

Koma, Y. *et al. Nuclear Materials and Energy*, 2017, 10, 35–41.

Following the 2011 accident at the Fukushima Daiichi nuclear power station (NPS), which is owned by Tokyo Electric Power Co., radioactive nuclides were released into the environment and heavily contaminated the NPS site. In this study, the contamination behaviour of radioactive nuclides in accumulated water, rubble, soil, and vegetation is discussed. Activity concentrations are converted to a 'transport ratio', which is the activity concentration ratio normalized using the activity in the source term for the nuclides of interest and a selected standard. The transport ratio of Sr to rubble and soil by way of air was approximately 10^{-2} to 10^{-3}, and the successive transport to accumulated water was comparable with Cs (except for the initial release). Transport of Pu, Am, and Cm was lower than for Sr regardless of the transport process (air or water), whereas those of I, Se, and Te were comparable or greater. Contamination with ^{3}H and ^{14}C was independent of ^{137}Cs, ^{90}Sr, and TRU nuclides and was likely a result of different transport process.

18/00169 Safety insights from forensics evaluations at Daiichi

Rempe, J. *et al. Nuclear Materials and Energy*, 2017, 10, 18–34.

Although it is clear that the accident signatures from each affected unit at the Fukushima Daiichi nuclear power station differ, much is not known about the end-state of core materials within these units. Some of this uncertainty can be attributed to a lack of information related to cooling system operation and cooling water injection. There is also uncertainty in the understanding of phenomena affecting: (a) in-vessel core damage progression during severe accidents in boiling water reactors (BWRs) and (b) accident progression after vessel failure (ex-vessel progression) for BWRs and pressurized water reactors (PWRs). These uncertainties arise due to limited full scale prototypic data. Similar to what occurred after the accident at Three Mile Island Unit 2, these Daiichi units offer the international community a means to reduce such uncertainties by obtaining prototypic data from multiple full-scale BWR severe accidents. Information obtained from Daiichi is required to inform decontamination and decommissioning activities, improving the ability of the Tokyo Electric Power Company (TEPCO) to characterize potential hazards and to ensure the safety of workers involved with clean-up activities. This paper reports initial results from the US Forensics Effort to utilize examination information obtained by TEPCO to enhance the safety of existing and future nuclear power plant designs. In this paper, three examples are presented in which examination information, such as visual images, dose surveys, sample evaluations, and muon tomography examinations, along with data from plant instrumentation, are used to obtain significant safety insights in the areas of component performance, fission product release and transport, debris end-state location, and combustible gas generation and transport. In addition to reducing uncertainties related to severe accident modelling progression, these insights confirm actions, such as the importance of water addition and containment venting, that are emphasized in updated guidance for severe accident prevention, mitigation, and emergency planning.

18/00170 Uranium as a renewable for nuclear energy

Degueldre, C. *Progress in Nuclear Energy*, 2017, 94, 174–186.

Uranium extraction is the first step of the nuclear fuel cycle. Currently, uranium is only extracted from solid ores such as uranium rich minerals (% level) or minerals such as phosphates (ppm level). For some years extraction of uranium from sea water (ppb level) has been the topic of investigations particularly in Japan due to its national interest. In the huge oceanic volume the amount of uranium is constant, regulated by its river input (soluble) and balanced by its scavenging (particulate) on the sea floor. This work shows that the uranium extraction with parsimony from sea water could be carried in a renewable way if its concentration remains quasi constant. Recommendations for the extraction with use of gel panels or with braid of fabric grafted by sorbing groups in high tide or oceanic pelagic current environments are suggested along with a reduction of the uranium consumption.

06 ELECTRICAL POWER SUPPLY AND UTILIZATION

Scientific, technical

18/00171 A one-day-ahead photovoltaic array power production prediction with combined static and dynamic on-line correction

Gulin, M. *et al. Solar Energy*, 2017, 142, 49–60.

This study develops and verifies a predictor-corrector method for a one-day-ahead photovoltaic array power production prediction. The most critical inputs to the prediction model are predictions of meteorological variables, such as solar irradiance components and the air temperature, which are the main sources of the power prediction uncertainty. Through a straightforward application of the weather forecast data sequence, photovoltaic array power production prediction is refreshed with the frequency of new forecasts generation by the meteorological service. It was shown that the prediction sequence quality can be significantly improved by using a neural-network-based corrector which takes into account near-history realizations of the prediction error. In this way it is possible to refresh the prediction sequence as soon as new local measurements become available. Except for predictions of meteorological variables, the prediction model itself is also a source of the prediction uncertainty, which is also taken into account by the proposed approach. The proposed predictor-corrector method is verified on real data over a 2-year time period. It is shown that the proposed approach can reduce the standard deviation of the power production prediction error up to 50%, but only for the first several instances of the prediction sequence (up to 6–8 h ahead) which are in turn the most relevant for real-time operation of predictive control systems that use the photovoltaic array power production prediction, like microgrid energy flows control or distribution network regulation.

18/00172 A single wire as all-inclusive fully functional supercapacitor

Kang, Q. *et al. Nano Energy*, 2017, 32, 201–208.

A key challenge in wire-shaped energy storage devices is their complete encapsulation for practical applications. Hence it is of great importance to design and fabricate an all-inclusive structure in which inner and outer current collectors, active materials, electrolyte and separator are all enclosed in a single wire structure. However, due to the surface area differences between the shell and core electrodes, the matching of the capacitance on both electrodes become a challenging task. The authors solved this problem by using multiple thin Ni wires with three-dimensional MnO_2-carbon nanotubes (CNTs)-graphene hybrids as the core electrode and a Ni tube as the shell electrode in a coaxial-cable supercapacitors structure. Within the seamless tubular electrode, all the necessary components are included and protected by the metal tube shell. The fully encapsulated single wire devices show a high area-

normalized capacitance of $31\,mF\,cm^{-2}$ at a current density of $0.29\,mA\,cm^{-2}$, comparable to the best cable devices with more exposed structures. Such devices are more suitable for applications by providing more mechanical stability and avoiding exposure and loss of electrolytes during operation.

18/00173 A small scale pressure retarded osmosis power plant: dynamics of the brackish effluent discharge along the coast

Stancanelli, L. M. *et al. Ocean Engineering*, 2017, 130, 417–428.

The feasibility of a small-scale pressure retarded osmosis (PRO) plant located along the eastern coast of Sicily in Italy is assessed by considering fresh water intake from a river and salt water intake from the sea. Firstly, PRO design methods are applied in order to estimate potential power production in terms of both the availability of water resources and of local salinity gradients. Secondly, the discharge dynamics of the brackish plant effluent in the coastal waters is investigated using an hydrodynamic model, taking into account wave–current interaction close to the river mouth. The results of the numerical simulations allow to identify the area affected by the brackish discharge, as a function of the nearshore wave climate conditions. Results show that the plume propagation is mainly controlled by the wave direction, whereas significant wave height and peak wave period have a minor influence. Plume hydrodynamics analysis is useful in optimizing the layout of the PRO plant in terms of the placement of the sea water intake and the effluent discharge, both of which should be properly located outside the surf-zone. Plume hydrodynamics analysis is also important for the evaluation of PRO plant impacts on the coastal saline concentration which may affect the local ecosystems.

18/00174 An analytical optimization of thermal energy storage for electricity cost reduction in solar thermal electric plants

González-Portillo, L. F. *et al. Applied Energy*, 2017, 185, 531–546.

Solar thermal electric (STE) plants can integrate thermal energy storage (TES) in order to generate electricity when the energy source (Sun radiation) has vanished. TES technology has become a very important asset for this type of renewable energy source, but it has induced a rise in electricity cost in many cases. One of the reasons is the need of larger solar fields as the TES capacity increases because the solar field has to provide thermal power both to generate electricity and to charge the storage. The economic effects of improving the plant performance seem to have some internal complexities that must be investigated covering the internal relations among the main parts of a STE plant: the solar field, the power block and the energy storage. This paper presents an analytical study of these relations aimed at deriving a better understanding of the cost/performance behaviour of STE plants. As the power block is a mature and commercial technology with well-established efficiencies and specific costs (in $/W, for instance), it has been taken as the reference element in modelling the plant. The other parts of the plant, i.e. the solar field and the energy storage, have been characterized in cost and energy management by a set of high-level parameters. Of course, a coarse definition cannot give very accurate results for a specific design, but it can be the guideline for the selection and sizing of a plant. It is worth noting that each type of solar thermal power plant has a different parametric scenario, corresponding to its essential design window. In this paper, comparisons among plants with different parametric scenarios are restricted to one-axis concentration solar fields, where the coarse model is easily characterized. The results show that the optimum plant configuration, in terms of TES capacity and solar field size, depends on the solar field and TES costs relative to power block cost. Moreover, it is shown that some parametric scenarios always lead to an increase in the cost of electricity when the energy storage capacity is enlarged. On the contrary, parametric scenarios associated to cheaper solar fields yield a much better economic result when TES is embodied in the plant. Additionally, TES efficiency is also identified as a parameter with high impact in the performance of the whole system. This result seems obvious, but the model gives numerical values that can help to optimize the selection process in a project. For instance, it is assessed that the lower the TES efficiency, the greater the relevance of reducing solar field costs is in order to obtain low electricity generation costs. As a general conclusion, the model points out that Fresnel-type solar fields are much better suited than parabolic trough collectors for integrating thermal energy storage. This implies that Fresnel plants present a higher potential to cover the peaks of electricity demand, which results into bigger profits.

18/00175 An inductor-free auto-power-management design built-in triboelectric nanogenerators

Zi, Y. *et al. Nano Energy*, 2017, 31, 302–310.

The triboelectric nanogenerator (TENG) has the output characteristics of high voltage but low current/charge-transfer, making its low efficiency in powering most of electronics. To address this problem, power management circuits consisting of coupled inductors or transformers are usually employed. Here the authors report an inductor-free, auto-power-management design based on automatic switches between serial-connected and parallel-connected capacitors in a rationally designed manner, so that the output voltage can be lowered and the output charge is enhanced in proportion. In conjunction to theoretical analysis, a TENG along with proof-of-concept power-management units as automatically driven by the triggering motion for TENG is fabricated, which improves the rate for charging a super-capacitor by five times. Compared to previous work, this power-management design shows advantages of capability for harvesting low power/frequency scale energy, high scalability, and light weight, which paves a new approach for achieving high-efficient portable TENG-based self-powered system.

18/00176 Analytical and numerical investigation on a new compact thermoelectric generator

Ming, T. *et al. Energy Conversion and Management*, 2017, 132, 261–271.

In order to improve the performance and maximize the efficiency of energy conversion of thermoelectric generator (TEG), a mathematical model to predict the maximum energy conversion efficiency of TEG is developed. Then, a new compact thermoelectric generator (C-TEG) and a dimensional optimized TEG (DO-TEG) are proposed in this article. The compact thermoelectric generator is designed via logical intersection angle selection and layout, thus to improve the electric performance per unit volume. Finally, the authors compared the output electric performance of C-TEG and traditional thermoelectric generator (T-TEG) and that of DO-TEG under design and off-design conditions via numerical simulations. The results indicate that C-TEG has an excellent electric performance whose voltage, power, and efficiency decrease slightly whereas the output voltage, work, and efficiency compared with that of T-TEG have been significantly improved, with the amplitude increasing with the increase of resistant value of external loads.

18/00177 Back-gated graphene anode for more efficient thermionic energy converters

Yuan, H. *et al. Nano Energy*, 2017, 32, 67–72.

Thermionic energy converters (TECs) are a direct heat-to-electricity conversion technology with great potential for high efficiency and scalability. However, space charge barrier in the inter-electrode gap and high anode work function are major obstacles toward realizing high efficiency. Here, the authors demonstrate for the first time a prototype TEC using a back-gated graphene anode, a barium dispenser cathode, and a controllable inter-electrode gap as small as $17\,\mu m$, which simultaneously addresses these two obstacles. This leads to an electronic conversion efficiency of 9.8% at cathode temperature of $1000\,^{\circ}C$, the highest reported by far. First it was demonstrated that electrostatic gating of graphene by a $20\,nm$ HfO_2 dielectric layer changes the graphene anode work function by $0.63\,eV$, as observed from the current–voltage characteristics of the TEC. Next, it was shown that the efficiency increases by a factor of 30.6 by reducing the gap from $1\,mm$ down to $17\,\mu m$, after a monolayer of Ba is deposited on graphene by the dispenser cathode. Finally, the authors show that electrostatic gating of graphene further reduces the graphene work function from 1.85 to $1.69\,eV$, leading to an additional 67% enhancement in TEC efficiency. Note that the overall efficiency using the back-gated graphene anode is 6.7 times higher compared with that of a TEC with a tungsten anode and the same inter-electrode gap.

18/00178 Development of Lyapunov redesign controller for microgrids with constant power loads

Hossain, E. *et al. Renewable Energy Focus*, 2017, 19–20, 49–62.

In microgrid applications, stability issues have been raised into a matter of concern due to the continually increasing modern electronic loads and inverter-based power electronic loads. In this paper, adopting storage system based load side compensation technique, a Lyapunov redesign controller is proposed to considerably improve the microgrid stability in the presence of constant power loads. Besides the controller design, the robustness analysis of the proposed Lyapunov redesign controller against parameter uncertainties is depicted. After that, the proposed Lyapunov redesign controller robustness against parametric uncertainties, frequency variations, and additive white Gaussian noise (AWGN) is presented. Later, performance of the PID and Lyapunov redesign controller is compared in the case of non-linearity, parameter uncertainties, and noise rejection to justify the selection of the Lyapunov redesign controller over the PID controller. Besides reckoning the necessary calculations, all of the results are verified in MATLAB/Simulink with the appreciable aftermath.

18/00179 Effective energy storage from a hybridized electromagnetic-triboelectric nanogenerator

Wang, X. and Yang, Y. *Nano Energy*, 2017, 32, 36–41.

This study reports on a hybridized electromagnetic-triboelectric nanogenerator including an electromagnetic generator (EMG) and a triboelectric nanogenerator (TENG) for simultaneously scavenging wind energy. The TENG can deliver a largest output power of about

1.7 mW under a loading resistance of 10 MΩ, while the EMG can deliver a largest output power of about 2.5 mW under a loading resistance of 1 kΩ. A power management circuit has been designed to store the produced energy from the TENG into a capacitor, resulting in the enhanced energy-storage efficiency of up to 112% as compared with that of using a traditional rectifier. The charging rate of the capacitor by using the TENG has been optimized by changing the inductance and the switching on/off time. As compared with the individual TENG or EMG, the hybridized nanogenerator has a much better ability for sustainably powering a temperature sensor, exhibiting the potential applications of hybridized nanogenerators in self-powered sensor systems.

18/00180 Electricity from wetlands: tubular plant microbial fuels with silicone gas-diffusion biocathodes

Wetser, K. *et al. Applied Energy*, 2017, 185, 642–649.

Application of the plant microbial fuel cell (PMFC) in wetlands should be invisible without excavation of the soil. The preferred design is a tubular design with the anode directly between the plant roots and an oxygen reducing biocathode inside the tube. Oxygen should be passively supplied to the cathode via a gas diffusion layer. In this research silicone was successfully used as gas diffusion layer. The objective of this research is to start-up an oxygen reducing biocathode *in situ* in a tubular PMFC applied in a *Phragmites australis* peat soil and a *Spartina anglica* salt marsh. PMFCs with a biocathode were successfully started in the peat soil. Oxygen reduction is clearly catalysed, likely by microorganisms in the cathodes, as the over-potential decreased resulting in an increased current density and cathode potential. The maximum daily average power generation of the best peat soil PMFC was 22 mW m^{-2}. PMFCs with a biocathode in the salt marsh only started with pure oxygen diffusion reaching a maximum daily average power generation of 82 mW m^{-2}. Both wetland PMFCs were successfully started with natural occurring microorganism in the anode and cathode. Calculations show that the power density can be increased by improving the PMFC design limiting crossover of oxygen and substrate.

18/00181 Energy conversion by 'T-shaped' cantilever type electromagnetic vibration based micro power generator from low frequency vibration sources

Siddique, A. R. M. *et al. Energy Conversion and Management*, 2017, 133, 399–410.

The design, development, and analyses of low-frequency vibration based T-shaped cantilever type electromagnetic micro power generators (EVMPGs) are presented in this paper. Four different configurations (configurations A–D) of EVMPGs were designed and fabricated and subsequently characterized using detailed experimental and limited analytical techniques. Configurations A and B consisted of a single and a double cylindrical moving magnets (NdFeB), respectively, while configuration C consisted of four rectangular moving magnets with respect to a fixed copper coil. In contrast, configuration D used a moving coil between four rectangular magnets with a back-iron bar. The open circuit RMS voltage output was observed to be a maximum from configuration D (98.2 mV at 6.29 Hz) with a base vibration acceleration of 0.8 m s^{-2}. Therefore, configuration D was selected for further experimental investigations, which included changing the back-iron bar thickness, changing the base acceleration level, and changing the air gap separation between the magnets in order to optimize this configuration. The maximum load RMS voltage and power outputs of configuration D were 105.4 mV and 1.35 mW at 6.29 Hz for load resistance 8.2 Ω and a base acceleration of 0.8 m s^{-2} with a 4.2 mm back-iron bar when the air gap between the magnets was 20 mm. Finally, a small portable EVMPG prototype was developed based on configuration D and was tested at different human movement conditions (i.e. walking, quick walking and running). The developed EVMPG prototype was capable of harvesting 35.2 mV and 0.22 mW at 7 Hz with load resistance 5.6 Ω for a base acceleration of 0.8 m s^{-2}.

18/00182 Energy flow modeling and optimal operation analysis of the micro energy grid based on energy hub

Ma, T. *et al. Energy Conversion and Management*, 2017, 133, 292–306.

The energy security and environmental problems impel people to explore a more efficient, environment friendly and economical energy utilization pattern. In this paper, the coordinated operation and optimal dispatch strategies for multiple energy system are studied at the whole micro energy grid level. To augment the operation flexibility of energy hub, the innovation sub-energy hub structure including power hub, heating hub and cooling hub is put forward. Basing on it, a generic energy hub architecture integrating renewable energy, combined cooling heating and power, and energy storage devices is developed. Moreover, a generic modelling method for the energy flow of micro energy grid is proposed. To minimize the daily operation cost, a day-ahead dynamic optimal operation model is formulated as a mixed integer linear programming optimization problem with considering the demand response. Case studies are undertaken on a community micro energy grid in four different scenarios on a typical summer day and the roles of renewable energy, energy storage devices and demand response are discussed separately. Numerical simulation results indicate that the proposed energy flow modelling and optimal operation method are universal and effective over the entire energy dispatching horizon.

18/00183 Energy management of DC microgrid based on photovoltaic combined with diesel generator and supercapacitor

Yin, C. *et al. Energy Conversion and Management*, 2017, 132, 14–27.

The microgrid is promoted as an economical and efficient energy system in which different renewable sources and storage are interconnected to meet the load power demand at any time. It can operate in on-grid and off-grid mode. Since the electrical contribution of each renewable energy source is dependent on the variation of its resource and the load power demand changes time to time, it is possible that the microgrid cannot generate enough electricity at some time. Thus, especially in off-grid mode, a diesel generator is needed as another backup power. However, due to the slow dynamic behaviour of the diesel generator start-up stage, the power quality is lowered down because of the shortage of power. Therefore, during the period of the diesel generator starting up, a supercapacitor is suggested to compensate the power balance because of its fast response and high power density. In addition, the supercapacitor can be also used to overcome the electrochemical storage limits like its state of charge and maximum current. This paper proposes a method for power balance control of a hybrid multisource DC microgrid system aiming to meet the load power demand with reliability and stabilizing the DC bus voltage. In order to realize this function, an experimental platform has been set up and the energy management strategy has been implemented into the control process. The experimental results show that the designed control strategy improves the DC microgrid dynamic and static performances under such operating conditions.

18/00184 Enhanced energy storage properties in $La(Mg_{1/2}Ti_{1/2})O_3$-modified $BiFeO_3$-$BaTiO_3$ lead-free relaxor ferroelectric ceramics within a wide temperature range

Zheng, D. and Zuo, R. *Journal of the European Ceramic Society*, 2017, 37, (1), 413–418.

A new ternary lead-free $(0.67\text{-}x)BiFeO_3$–$0.33BaTiO_3$–$xLa(Mg_{1/2}Ti_{1/2})O_3$ ferroelectric ceramic exhibited an obvious evolution of dielectric relaxation behaviour. A significantly enhanced energy-storage property was observed at room temperature, showing a good energy-storage density of 1.66 J/cm^3 at 13 kV/mm and a relatively high energy-storage efficiency of 82% at $x = 0.06$. This was basically ascribed to the formation of a slim polarization-electric field hysteresis loop, in which a high saturated polarization P_{max} and a rather small remnant polarization P_r were simultaneously obtained. Particularly, its energy storage properties were found to depend weakly on frequency (0.2–100 Hz), and also to exhibit a good stability against temperature (25–180 °C). The achievement of these characteristics was attributed to both a rapid response of the electric field induced reversible ergodic relaxor to long-range ferroelectric phase transition and a typical diffuse phase transformation process in the dielectric maxima.

18/00185 Examination of scintillator-photovoltaic cell-based spent fuel radiation energy conversion for electricity generation

Lee, H. and Yim, M.-S. *Progress in Nuclear Energy*, 2017, 94, 46–54.

Using computational models, this research examined electricity generation from spent nuclear fuel and its possible uses. The proposed approach was based on converting gamma radiation energy into electricity using scintillators and photovoltaic cells. The work includes performing gamma radiation environment analysis around spent fuel, scintillated photon analysis, and photovoltaic cell analysis for electricity generation. The OrigenArp code was used for gamma radiation environment analysis and the MCNPX 2.7.0 code was used for analysing scintillation process. For the scintillated photon analysis and photovoltaic cell analysis, a new simulation model was developed and validated based on comparison with experimental data. The effect of self-absorption and radiation damage within the scintillator was described by using experimental data. Based on using 14 energy conversion system units in a spent fuel storage pool in a PWR with $CdWO_4$ as scintillator and SiO_2 as photovoltaic cell, generation of electric energy was estimated to range between a few hundred watts and a few watts depending on the cooling time. The estimated amount of electric power generation from spent fuel energy conversion was not enough for large-scale applications. But the converted electric power could be utilized as emergency power source in an operating nuclear power plant for various detection and monitoring purposes and for the support of spent fuel pool cooling pump operations.

18/00186 Exergy analysis of a combined cooling, heating and power system integrated with wind turbine and compressed air energy storage system

Mohammadi, A. *et al. Energy Conversion and Management*, 2017, 131, 69–78.

Utilizing renewable energies is the promising solution to the environmental problems which are brought about due to fossil fuel consumption. The fact that these kinds of energies are intermittent can be overcome with using energy storage systems. Wind energy coupled with compressed air energy storage systems is one of the best candidates in this respect. The main objective of this paper is to study the integration of this system with a combined cooling, heating and power cycle comprised of a gas turbine, an organic Rankine cycle and an absorption refrigeration system. Energy and exergy analyses are applied to the system and the effect of key parameters on the system performance are analysed. The results show that under design condition, the system can generate 33.67 kW electricity, 2.56 kW cooling and 1.82 ton per day hot water with a round trip energy efficiency of 53.94%. Also exergy analysis reveals that wind turbine, combustion chamber and compress air storage system have the highest amount of exergy destruction respectively. Finally, sensitivity analysis shows that parameters related to gas turbine are the most prominent parameters of the system which can change performance of the system considerably.

18/00187 Experimental demonstration of a novel approach to increase power conversion potential of a hydrocarbon fuelled, portable, thermophotovoltaic system

Kang, X. and Veeraragavan, A. *Energy Conversion and Management*, 2017, 133, 127–137.

A novel, compact mesoscale thermophotovoltaic (TPV) power generating system using a combination of porous media combustion and a simple band-pass filtering method has been proposed and experimentally studied. The novelty in this work is the idea of harvesting the heat produced in the microcombustor via the silicon carbide (SiC) porous media which becomes an effective radiator owing to its high emissivity. This is then combined with wafers that have a high optical transmissivity in the part of the spectrum that is useful for power conversion using the TPV system. Here the authors utilized two combustor wafers (silicon and quartz) with suitable thermal and optical properties. Quartz having a high transmissivity of 0.9 compared to silicon (<0.6) proved to be superior in performance when combined with the porous media combustion for TPV power generation. To further illustrate the combination of effects, the authors also performed experiments in which porous media was not inserted in the combustor and the radiation was effectively from the hot combustor walls. In this case, silicon which has a higher emissivity than the quartz performs better. Overall the TPV power generation was SiC + quartz > SiC + Si < pure Si walls > pure quartz walls.

18/00188 Experimental investigation and exergy analysis on thermal storage integrated micro-cogeneration system

Johar, D. K. *et al. Energy Conversion and Management*, 2017, 131, 127–134.

This paper describes the performance of thermal storage integrated micro-cogeneration system based on single cylinder diesel engine. In addition to electricity generated from genset, waste heat from hot exhaust of diesel engine was used to heat water in a double pipe heat exchanger of 67.70 cm length with inside tube diameter of 3.81 cm and outside tube diameter of 5.08 cm. Additionally, a latent heat thermal energy storage system was also integrated with this cogeneration system. A shell and tube type heat exchanger of 346 mm diameter and 420 mm height with 45 tubes of 18 mm diameter each was designed and fabricated, to store thermal energy, in which Erythritol ($C_4H_{10}O_4$) was used as phase changing material. The test results show that micro capacity (4.4 kW), stationary, single cylinder, diesel engine can be successfully utilized to simultaneously produce power as well as heating, and to also store thermal energy. Slight decrease in engine performance was observed when double pipe heat exchanger and latent heat thermal energy storage system was integrated with engine but the amount of energy which could be recovered was significant. Maximum percentage of energy saved was obtained at a load of 3.6 kW and was 15.2%.

18/00189 High-performance nickel-cobalt-boron material for an asymmetric supercapacitor with an ultrahigh energy density

Chen, R. *et al. Journal of Power Sources*, 2017, 341, 75–82.

Nickel–cobalt–borons (Ni–Co–B) are synthesized using a facile and cost-effective reduction method. The effects of Ni/Co molar ratios and crystallinity on its supercapacitive performance are systematically investigated. It was found that nickel-cobalt-borons with the Ni/Co ratio being 2:1 and amorphous structure manifest the optimum specific capacitance of 2226.96 F/g at a current density of 1 A/g and still remain 1879.2 F/g with a high discharge current density of 20 A/g. An asymmetric supercapacitor device (ASC) has been fabricated with Ni–Co–B as the positive electrode and commercial activated carbon (CAC) as the negative electrode material. The Ni–Co–B//CAC delivers an ultrahigh energy density of 66.40 Wh/kg at a power density of 788.91 W/kg. This ASC remains 85.76% of its initial capacitance even after 5000 charge–discharge cycles. The results demonstrate that amorphous Ni–Co–B material is a promising candidate for energy storage application.

18/00190 High-performance reverse electrowetting energy harvesting using atomic-layer-deposited dielectric film

Yang, H. *et al. Nano Energy*, 2017, 31, 450–455.

Reverse electrowetting-on-dielectric (REWOD), which is a novel technology for energy harvesting, was demonstrated by depositing Al_2O_3 via atomic layer deposition (ALD). Specifically, thin layers of Al_2O_3 about 100 nm-thick were successfully formed by ALD to obtain dense films with high capacitances. REWOD with the ALD Al_2O_3 thin films exhibited high performances under low-voltage and low-excitation-frequency conditions. The maximum power density was 11 mW/cm^2 with a DC bias of 24 V and an external excitation frequency of 2 Hz. Moreover, ALD and sputtered thin films were compared by investigating their capacitances and leakage current densities. Due to the differences between the film densities and growth methods, the ALD thin films exhibited higher capacitances and lower leakage current densities. It was also determined that the leakage current affects the REWOD energy harvesting performance. By analysing these features, it was confirmed that ALD thin films are suitable for REWOD energy harvesting.

18/00191 Hysteretic behavior of contact force response in triboelectric nanogenerator

Seol, M.-L. *et al. Nano Energy*, 2017, 32, 408–413.

The hysteretic behaviour of contact force response in a triboelectric nanogenerator is analysed as the output performance in response to the applied contact force is found to be dependent on previous contact force history. The counterclockwise hysteresis curve of the contact force versus output power originates from the asymmetric time constant between triboelectric charging and natural discharging, because the charges due to contact electrification do not immediately disappear but gradually decay over a period of hours. Therefore, a low contact force followed immediately after a high contact force results in enhanced output performance but not the reverse order. However, if the intermission time becomes too long, the benefit due to charge balance gets degraded. The experimental results on sweep range and discharging time dependencies agree well with theoretical expectations.

18/00192 Model predictive control power management strategies for HEVs: a review

Huang, Y. *et al. Journal of Power Sources*, 2017, 341, 91–106.

This paper presents a comprehensive review of power management strategy (PMS) utilized in hybrid electric vehicles (HEVs) with an emphasis on model predictive control (MPC) based strategies for the first time. Research on MPC-based power management systems for HEVs has intensified recently due to its many inherent merits. The categories of the existing PMSs are identified from the latest literature, and a brief study of each type is conducted. Then, the MPC approach is introduced and its advantages are discussed. Based on the acquisition method of driver behaviour used for state prediction and the dynamic model used, the MPC is classified and elaborated. Factors that affect the performance of the MPC are put forward, including prediction accuracy, design parameters, and solvers. Finally, several important issues in the application of MPC-based power management strategies and latest developing trends are discussed. This paper not only provides a comprehensive analysis of MPC-based power management strategies for HEVs but also puts forward the future and emphasis of future study, which will promote the development of energy management controller with high performance and low cost for HEVs.

18/00193 Modeling reliability of power systems substations by using stochastic automata networks

Šnipas, M. *et al. Reliability Engineering & System Safety*, 2017, 157, 13–22.

In this paper, stochastic automata networks (SANs) formalism to model reliability of power systems substations is applied. The proposed strategy allows reducing the size of state space of Markov chain model and simplifying system specification. Two case studies of standard configurations of substations are considered in detail. SAN models with different assumptions were created. SAN approach is compared with exact reliability calculation by using a minimal path set method. Modelling results showed that total independence of automata can be assumed for relatively small power systems substations with reliable equipment. In this case, the implementation of Markov chain model by a using SAN method is a relatively easy task.

18/00194 Nano-micro-porous skutterudites with 100% enhancement in ZT for high performance thermoelectricity

Khan, A. U. *et al. Nano Energy*, 2017, 31, 152–159.

Increasing energy demands require new materials, e.g. thermoelectrics, for efficient energy conversion of fossil fuels. However, their low figure of merit (ZT) limits widespread applications. Nanostructuring has been an effective way of lowering the thermal conductivity. However, grain growth at elevated temperature is still a big concern, for otherwise expected to be long-lasting thermoelectric generators. Here, the authors report a porous architecture containing nanometre to micrometre size irregularly shaped and randomly oriented pores, scattering a wide spectrum of phonons without employing the conventional rattling phenomenon. Lattice thermal conductivity reaches the phonon glass limit. This design yields >100% enhancement in ZT, as compared to the pristine sample. An unprecedented and very promising ZT of 1.6 is obtained for Co23.4Sb69.1Si1.5Te6.0 alloy, by far the highest ZT ever reported for unfilled skutterudites, with further benefits, i.e. rare-earth-free and improved oxidation resistance enabling simple processing.

18/00195 On the relation between battery size and PV power ramp rate limitation

Makibar, A. *et al. Solar Energy*, 2017, 142, 182–193.

Photovoltaic (PV) power fluctuations caused by clouds are leading operators of grids with high renewable energy penetration rates to impose ramp rate limitations. Costly battery energy storage systems are used for fulfilling these regulations but the question of the power and energy requirements for accomplishing them has not been fully answered. This work analyses the effects of reducing the size of a battery designed to absorb every fluctuation by taking into consideration, both, the fluctuation occurrence and the penalties in case of non-compliance of a given prescribed ramp-rate limitation. A theoretical analysis was carried out in order to assess the relation between size reduction and ramp rate compliance, obtaining as result a model for predicting the probability of non-compliances with a reduced battery. Additionally, the battery size reduction analysis was applied to the particular grid code currently proposed for Puerto Rico, creating new tools for selecting a battery with reduced power and energy capacity.

18/00196 Optimal day ahead scheduling of combined heat and power units with electrical and thermal storage considering security constraint of power system

Kia, M. *et al. Energy*, 2017, 120, 241–252.

The use of combined heat and power (CHP) with an overall efficiency from 70% to 90% is one of the most effective solutions to optimize the energy consumption. Mainly due to interdependence of the power and heat in these systems, the optimal operation of CHP systems is a complex optimization problem that needs powerful solutions. This paper addresses optimal day-ahead scheduling of CHP units with electric storage systems and thermal storage systems considering security constraints. Basically, the optimal scheduling of CHP units problem is a mixed integer non-linear problem with many stochastic and deterministic variables. In this paper, linearization techniques are adopted to linearize equations and a two-stage stochastic mixed-integer linear programming model is utilized to solve the problem. The first stage models behaviour of operation parameters and minimizes the operation costs meanwhile the second stage considers the system's stochastic contingency scenarios. The proposed method is applied to 18-bus, 24-bus IEEE test systems. The effectiveness of the proposed algorithm has been investigated.

18/00197 Optimal placement and sizing of distributed generators for voltage-dependent load model in radial distribution system

Kumar, M. *et al. Renewable Energy Focus*, 2017, 19–20, 23–37.

The power demand is expanding consistently, which results in the increment of power losses and dropped voltage of the distribution system. Integrating distributed generation (DG) substantially reduces the power loss and increases the voltage profile. In order to get maximum compensation from DG, it ought to be coordinated with optimal placement and sizing. In this paper, an extensive investigation is exhibited for the optimal placement and sizing of different types of one and multiple DGs with existing and increased loads. Electrical load growth is modelled for the base year and next three years with the predetermined load growth. In practice, the distribution system has different types of consumers, assuming constant power load model will lead to inappropriate results. Thus, five different types of load models such as constant, residential, industrial, commercial and mixed loads are considered. Three distinct sorts of DGs were chosen for this study, that is, active, reactive and combination of active–reactive power DG. The proposed study has been applied to the IEEE 33 radial distribution system with basic particle swarm optimization algorithm. The results reveal that combination of active–reactive power DG is giving better results for power loss reduction and voltage profile improvement, compared to the other DG types.

18/00198 Overview on recent developments in energy storage: mechanical, electrochemical and hydrogen technologies

Amirante, R. *et al. Energy Conversion and Management*, 2017, 132, 372–387.

Energy production is changing in the world because of the need to reduce greenhouse gas emissions, to reduce the dependence on carbon/fossil sources and to introduce renewable energy sources. Despite the great amount of scientific efforts, great care to energy storage systems is necessary to overcome the discontinuity in the renewable production. A wide variety of options and complex characteristic matrices make it difficult and so in this paper the authors show a clear picture of the available state-of-the-art technologies. The paper provides an overview of mechanical, electrochemical and hydrogen technologies, explaining operation principles, performing technical and economic features. Finally a schematic comparison among the potential utilizations of energy storage systems is presented.

18/00199 Potential reduction of carbon dioxide emissions from the use of electric energy storage on a power generation unit/organic Rankine system

Mago, P. J. and Luck, R. *Energy Conversion and Management*, 2017, 133, 67–75.

This paper evaluates the potential carbon dioxide emissions reduction from the implementation of electric energy storage to a combined power generation unit and an organic Rankine cycle relative to a conventional system that uses utility gas for heating and utility electricity for electricity needs. Results indicate that carbon dioxide emission reductions from the operation of the proposed system are directly correlated to the ratio of the carbon dioxide emission conversion factor for electricity to that of the fuel. The location where the system is installed also has a strong influence on the potential of the proposed system to save carbon dioxide emissions. Finally, it is shown that by using carbon emissions cap and trade programs, it is possible to establish a frame of reference to compare/exchange operational cost gains with carbon dioxide emission reductions/gains.

18/00200 Progress in dynamic simulation of thermal power plants

Alobaid, F. *et al. Progress in Energy and Combustion Science*, 2017, 59, 79–162.

While the conventional design of thermal power plants is mainly focused on high process efficiency, market requirements increasingly target operating flexibility due to the continuing shift towards renewables. Dynamic simulation is a cost-efficient tool for improving the flexibility of dispatchable power generation in transient operation such as load changes and start-up procedures. Specific applications include the optimization of control structures, stress assessment for critical components and plant safety analysis in malfunction cases. This work is a comprehensive review of dynamic simulation, its development and application to various thermal power plants. The required mathematical models and various components for description the basic process, automation and electrical systems of thermal power plants are explained with the support of practical example models. The underlying flow models and their fundamental assumptions are discussed, complemented by an overview of commonly used simulation codes. Relevant studies are summarized and placed in context for different thermal power plant technologies: combined-cycle power, coal-fired power, nuclear power, concentrated solar power, geothermal power, municipal waste incineration and thermal desalination. Particular attention is given to those studies that include measurement validation in order to analyse the influence of model simplifications on simulation results. In conclusion, the study highlights current research efforts and future development potential of dynamic simulation in the field of thermal power generation.

18/00201 Scalable single crystalline PMN-PT nanobelts sculpted from bulk for energy harvesting

Chen, Y. *et al. Nano Energy*, 2017, 31, 239–246.

Microelectromechanical systems (MEMS) incorporating piezoelectric elements enable highly sensitive sensors/actuators and effective energy harvesting. The development of a facile method for fabricating high-quality, deterministically positioned piezoelectric nanostructures provides new opportunities to build MEMS devices with dramatically higher performance. Piezoelectric materials with superior piezoelectric response, such as the relaxor ferroelectric $Pb(Mg,Nb)O_3$-$PbTiO_3$ (PMN-PT) represents a particularly interesting active material that functions as sensors/actuators and energy harvesters. Bottom-up synthesis of PMN-PT nanostructure suffers from polycrystallinity and stoichiometric deficiency. Yet, another main challenge is the deterministic positioning, aligning and integrating of as-synthesized nanostructures into functional arrays, in a similar manner to top-down strategies. Here, the authors fabricated scalable ordered single crystalline PMN-PT nanobelt (NB) arrays via a versatile top-down method. These NBs arrays, selectively sculpted from a single crystal

bulk preserve well ferroelectric properties and exhibit the highest reported piezoelectric coefficient (~677 pm/V). A flexible PMN-PT NB harvester was demonstrated based on these single crystalline NBs. The maximum output voltage and current reach ~6.0 V and ~102 μA, respectively under a 0.2% strain agitation. The result paves the way towards real application for top-down fabricated PMN-PT NBs as nanogenerators.

18/00202 Significantly enhanced energy storage performance promoted by ultimate sized ferroelectric $BaTiO_3$ fillers in nanocomposite films

Hao, Y. *et al. Nano Energy*, 2017, 31, 49–56.

Polymer nanocomposite that consists of dispersed particle fillers and a flexible polymer matrix shows comprehensive excellent dielectric properties and thus is considered as promising dielectric layers in high-performance energy-storage capacitors. However, the commonly employed high permittivity particle fillers cause inevitable dielectric strength deterioration and seriously impede the energy density and reliability of the nanocomposite. To solve this problem, ultimate sized ferroelectric nanofillers, 6.9 nm $BaTiO_3$ nanocrystals, are introduced into a poly(vinylidene fluoride-co-hexafluoro propylene) (PVDF-HFP) polymer matrix to realize both the high dielectric constant and enhanced breakdown strength. The influence of nanoparticle fraction on the microstructure and dielectric properties of the composite films is investigated. Compared to the polymer-ceramic composites with coarse particle fillers, significantly enhanced breakdown strengths (≥330 kV/mm) are observed in the nanocomposite films containing 10–40 vol.% $BaTiO_3$ nanofillers. In consequence, a maximal discharged energy density of 9.7 J/cm^3 is obtained, which confirms that these ultimate sized nanocrystals can perform as superior high permittivity fillers in the nanocomposites for energy storage applications.

18/00203 Solar polygeneration for electricity production and desalination: case studies in Venezuela and northern Chile

Mata-Torres, C. *et al. Renewable Energy*, 2017, 101, 387–398.

In this study, a polygeneration system incorporating concentrating solar power (CSP) integrated with a desalination plant is investigated. Parabolic trough collectors (PTC) and multi-effect distillation (MED) technologies are considered, and a transient system model has been simulated using the TRNSYS software. Two alternative desalination integration options and two potential locations in Venezuela and Chile with electricity and freshwater supply problems were selected and studied. Chile has also set a 20% target for non-conventional renewable energy production by 2025; therefore a polygeneration system coupled with desalinization plant is aligned with the needs of both countries. The results show that the CSP polygeneration plant can provide electricity and freshwater to more than 85,000 inhabitants at a reasonable cost; however the costs and feasibility depend principally on the irradiation, the location of plant with respect to the sea, and the specific conditions of each country. With the projected costs expected to decrease, it could be feasible to develop a CSP polygeneration plant in either country. For the Chilean case, LEC and LWC can be reduced to competitive prices if the initial PTC investment cost could be reduced by 15% for the Chilean case, and by 25% for the Venezuelan case.

18/00204 Strong and anisotropic magnetoelectricity in composites of magnetostrictive Ni and solid-state grown lead-free piezoelectric BZT–BCT single crystals

Palneedi, H. *et al. Journal of Asian Ceramic Societies*, 2017, 5, (1), 36–41.

Aimed at developing lead-free magnetoelectric (ME) composites with performances as good as lead (Pb)-based ones, this study employed (001) and (011) oriented $82BaTiO_3$-$10BaZrO_3$-$8CaTiO_3$ (BZT–BCT) piezoelectric single crystals, fabricated by the cost-effective solid-state single crystal growth (SSCG) method, in combination with inexpensive, magnetostrictive base metal nickel (Ni). The off-resonance, direct ME coupling in the prepared Ni/BZT–BCT/Ni laminate composites was found to be strongly dependent on the crystallographic orientation of the BZT–BCT single crystals, as well as the applied magnetic field direction. Larger and anisotropic ME voltage coefficients were observed for the composite made using the (011) oriented BZT–BCT single crystal. The optimized ME coupling of 1 V/cm Oe was obtained from the Ni/(011) BZT–BCT single crystal/Ni composite, in the d_{32} mode of the single crystal, when a magnetic field was applied along its [100] direction. This performance is similar to that reported for the Ni/$Pb(Mg_{1/3}Nb_{2/3})O_3$-$Pb(Zr,Ti)O_3$ (PMN–PZT) single crystal/Ni, but larger than that obtained from the Ni/$Pb(Zr,Ti)O_3$ ceramic/Ni composites. The results of this work demonstrate that the use of lead-free piezoelectric single crystals with special orientations permits the selection of desired anisotropic properties, enabling the realization of customized ME effects in composites.

18/00205 Systematic study on structural and electronic properties of diamine/triamine functionalized graphene networks for supercapacitor application

Song, B. *et al. Nano Energy*, 2017, 31, 183–193.

In this paper, a series of diamine/traimine molecules were selected to make different functionalized graphene networks using a facile two-step hydrothermal method. The molecular level grafting of amines to graphene surface via covalent bonds was confirmed by FTIR and XPS. XRD patterns revealed that these amine molecules served as molecular spacers to enlarge the interlayer spacing and the specific surface area. Upon functionalization, the interlayer spacing values varied from 0.84 to 1.23 nm, and the spacing was found to change negligibly after the GO reduction, implying the high stability of the 3D graphene nanostructure. The influence of chain conformation and degree of functionalization on molecular spacing was also discussed. The as-fabricated graphene composite exhibited an improved capacitance in aqueous and organic electrolytes with less than 10% capacitance decay during 10,000 charge/discharge cycles and fast ionic diffusion features. The composite also delivered a maximum capacitance of 119 F/g in ionic liquid electrolyte with an ultrahigh energy density of 51 Wh/kg and slow self-discharge rate. Furthermore, computational study was performed to model the electron distribution and band gap structures of graphene networks. The use of aliphatic amine spacers could better elucidate the correlation between spacing effect and electrical double-layer capacitance.

18/00206 Utilizing primary energy savings and exergy destruction to compare centralized thermal plants and cogeneration/trigeneration systems

do Espirito Santo, D. B. and Gallo, W. L. R. *Energy*, 2017, 120, 785–795.

Rising energy conversion processes efficiencies reduces CO_2 emissions and global warming implications. Decentralized electricity production through cogeneration/trigeneration systems can save primary energy if it operates with high efficiency. High efficiency is obtained when the system produces electricity and a substantial amount of the energy rejected by the prime mover is used to meet site thermal demands. Environmental concerns and international agreements are directing governments of different countries to incentive high efficiency solutions. Centralized thermal plants and cogeneration/trigeneration efficiency are compared through efficiency indicators using the first law of thermodynamics and the second law of thermodynamics. This paper proposes the use of the primary energy savings analysis and the exergy destruction analysis to compare decentralized power production through cogeneration/trigeneration systems and centralized thermal plants. The analysis concluded that both methods achieve the same results if the thermal efficiency indicator is used to compare the methods. The analysis also revealed that trigeneration systems with the same energy input are comparable with quite different thermal efficiency centralized thermal plants. Case 1 is comparable to a 53% thermal efficiency power plant and case 2 is comparable to a 77% thermal efficiency power plant.

Economics, policy, supplies, forecasts

18/00207 A comprehensive sequential review study through the generation expansion planning

Sadeghi, H. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 1369–1394.

The generation expansion planning (GEP) problem involves the determination of types, location and construction time of new generation technologies which should be added to the existing system in order to meet the growing demand over a planning horizon. It is a vital issue due to electricity-dependent aspect of everyday life as well as most production and service systems in society. Over the past few decades, the GEP has experienced multifarious changes resulting in emerging a multitude of new models and solving methods. In this context, many studies have been carried out to achieve optimal expansion strategies with respect to the different energy-related issues, such as electricity market, uncertainties, low carbon economy requirements, distributed generation, renewable sources, energy policies, demand-side programs, and so on. In pursuance of finding out further research ideas in the field of GEP and identify less-addressed areas, a need for a comprehensive review of accomplished studies has been felt. By reviewing almost all aspects that have been considered in the GEP as yet, the present paper provides a detailed classification of a large number of done GEP studies. Reviewing results provide useful insights into the future of GEP research activities.

18/00208 A comprehensive study of economic unit commitment of power systems integrating various renewable generations and plug-in electric vehicles

Yang, Z. *et al. Energy Conversion and Management*, 2017, 132, 460–481.

Significant penetration of renewable generations (RGs) and mass roll-out of plug-in electric vehicles (PEVs) will pay a vital role in delivering the low carbon energy future and low emissions of greenhouse gases (GHG) that are responsible for the global climate change. However, it is of considerable difficulties to precisely forecast the undispatchable and intermittent wind and solar power generations. The uncoordinated charging of PEVs imposes further challenges on the unit commitment in modern grid operations. In this paper, all these factors are comprehensively investigated for the first time within a novel hybrid unit commitment framework, namely UCsRP, which considers a wide range of scenarios in renewable generations and demand side management of dispatchable PEVs load. UCsRP is however an extremely challenging optimisation problem not only due to the large scale, mixed integer and non-linearity, but also due to the double uncertainties relating to the renewable generations and PEV charging and discharging. In this paper, a meta-heuristic solving tool is introduced for solving the UCsRP problem. A key to improve the reliability of the unit commitment is to generate a range of scenarios based on multiple distributions of renewable generations under different prediction errors and extreme predicted value conditions. This is achieved by introducing a novel multi-zone sampling method. A comprehensive study considering four different cases of unit commitment problems with various weather and season scenarios using real power system data are conducted and solved, and smart management of charging and discharging of PEVs are incorporated into the problem. Test results confirm the efficacy of the proposed framework and new solving tool for UCsRP problem. The economic effects of various scenarios are comprehensively evaluated and compared based on the average economic cost index, and several important findings are revealed.

18/00209 A meta-analysis on the price elasticity of energy demand

Labandeira, X. *et al. Energy Policy*, 2017, 102, 549–568.

Price elasticities of energy demand have become increasingly relevant in estimating the socio-economic and environmental effects of energy policies or other events that influence the price of energy goods. Since the 1970s, a large number of academic papers have provided both short and long-term price elasticity estimates for different countries using several models, data and estimation techniques. Yet the literature offers a rather wide range of estimates for the price elasticities of demand for energy. This paper quantitatively summarizes the recent, but sizeable, empirical evidence to facilitate a sounder economic assessment of (in some cases policy-related) energy price changes. It uses meta-analysis to identify the main factors affecting short and long term elasticity results for energy, in general, as well as for specific products, i.e. electricity, natural gas, gasoline, diesel and heating oil.

18/00210 A method for distinguishing appliance, lighting and plug load profiles from electricity 'smart meter' datasets

George, D. and Swan, L. G. *Energy and Buildings*, 2017, 134, 212–222.

In the Canadian residential sector, the end-uses of appliances, lighting, and plug loads (ALP) account for 16% of total end-use energy consumption. In an effort to reduce the impacts of this energy consumption, electricity technologies such as solar photovoltaics and smart appliances are being adopted. Evaluation of their performance requires an understanding of residential electricity use patterns. Building simulation tools can estimate the time-step performance of such technologies, but require accurate and representative ALP electricity profiles as an input. Sub-metered datasets lack in quantity and thus overall representativeness of the sector. Meanwhile, large, representative datasets are becoming available through electricity smart-metering programs, but usually consist only of whole-house electricity load and lack summary household characteristics (e.g. occupancy, floor space, appliance descriptions). However, homes which are not electrically heated (space, water) or cooled may function as ALP load profiles for simulation. This research addresses these loads with a new method of distinguishing non-electrically heated and cooled homes from a broad dataset of whole-house profiles. The method originates from a comparison of two electricity load datasets: (i) 'smart-meter' 15-min time-step whole-house data for 160 homes spanning three years, and (ii) 'sub-metered' 1-min time-step data for 23 residential homes. This comparison also speaks to the usefulness of whole-house electricity smart-meter information to building performance simulation.

18/00211 A multi-region load dispatch model for the long-term optimum planning of China's electricity sector

Guo, Z. *et al. Applied Energy*, 2017, 185, 556–572.

Future development of China's electricity system will not only need to consider generation capacity needed to meet demand but also economic and flexible technologies to meet peak demand and integrate increasing volumes of intermittent renewable generation. This paper describes research in which a multi-region dispatch model was established and analysis performed to gain insights into optimal choices for the development of China's electricity sector. The model reflected China's regional electricity demand profiles, its natural resource distribution, its inter-regional electricity transmission network, performance characteristics of different electricity generating technologies, and temporal electricity demand variations. The case study included a cap-and-trade carbon mitigation scheme to enable direct comparison with previous studies that lacked the temporal element considerations. The results highlighted the importance of considering even short-term temporal variations when planning the long-term development of electricity systems. They also demonstrated how natural gas combined cycle turbines are well suited to providing peak-demand regulation capability. Whilst, the analysis indicates that coal-fired plants are set to continue to play a significant role through out to 2050. The modelling also confirms the deployment of renewable energy in the long-term future and as a result the requirement of flexible generation to maintain stability and integrity.

18/00212 A rough multi-factor model of electricity spot prices

Bennedsen, M. *Energy Economics*, 2017, 63, 301–313.

This study introduces a new continuous-time mathematical model of electricity spot prices which accounts for the most important stylized facts of these time series: seasonality, spikes, stochastic volatility, and mean reversion. Empirical studies have found a possible fifth stylized fact, roughness, and the approach used here explicitly incorporates this into the model of the prices. This setup generalizes the popular Ornstein–Uhlenbeck-based multi-factor framework and allows us to perform statistical tests to distinguish between an Ornstein–Uhlenbeck-based model and a rough model. Further, through the multi-factor approach, the authors account for seasonality and spikes before estimating – and making inference on – the degree of roughness. This is novel in the literature and the authors present simulation evidence showing that these precautions are crucial for accurate estimation. Lastly, they estimate their model on recent data from six European energy exchanges and find statistical evidence of roughness in five out of six markets. As an application of this model, the authors show how, in these five markets, a rough component improves short-term forecasting of the prices.

18/00213 Biomass sorghum production risk assessment analysis: a case study on electricity production in the Po Valley

Serra, P. *et al. Biomass and Bioenergy*, 2017, 96, 75–86.

The risk associated to the production of biomass sorghum (*Sorghum bicolor* (L.) Moench) to feed a power plant in the Po Valley (Italy) was studied with a modelling approach. Available biomass was modelled by CropSyst, coupled to a 'sorghum haying model', using three sorghum genotypes, of contrasting earliness (early, medium-late and late), on a mosaic of virtual farms created in the target cropping area. The energy performance, from cradle to farm gate, of the biomass production system was performed calculating energy return on investment (EROI), net energy gain (NEG) and energy use efficiency (EUE). The highest baled biomass (14.0 Mg DM $ha^{-1}y^{-1}$) was obtained with the early maturity type that had less haymaking failures (6.9%), followed by the late and medium-late genotypes. As a consequence, the early maturity type had the highest probability of exceeding the biomass needs of the power plant on a cropping area of 4222 ha. The early genotype also had the highest EROI (14.8) and NEG (205.6 GJ $ha^{-1}y^{-1}$) and the lowest EUE (1.06 GJ Mg^{-1} DM y^{-1}). To achieve a 0.5 probability to exceed the target biomass production, the area to be cultivated should be 4558, 5160 and 4962 ha for the early, medium-late and late genotypes, respectively.

18/00214 Climate change impact and resilience in the electricity sector: the example of Austria and Germany

Totschnig, G. *et al. Energy Policy*, 2017, 103, 238–248.

The purpose of this paper is to investigate the resilience of possible future electricity and heating systems in regard to climate change and fuel price shocks. The dynamical simulation model HiREPS of the Austrian and German electricity, heating and cooling sectors was used for this analysis. The electricity generation cost and changes in the required secured capacity were used as indicators for the resilience of the energy system. The results show, that the analysed changes in the natural gas price have larger impact on the electricity generation cost than weather variability between different years or climate change. Especially the fossil fuel based scenario showed high sensitivity to the gas price. Analysis of the required secured capacity shows, that in the last quarter of the twenty-first century the annual maximum residual loads are growing and are dominated by strong cooling demand peaks.

Promoting passive cooling options, efficient building designs and options for a controlled down regulation of cooling devices seems to be advisable to avoid installing large thermal power plant backup capacities. The evaluated climate model simulations show only small changes in photovoltaic, wind and hydro power generation for 2051–2080 in Austria and Germany.

18/00215 Demand management to mitigate impacts of plug-in electric vehicle fast charge in buildings with renewables

Sehar, F. *et al. Energy*, 2017, 120, 642–651.

Plug-in electric vehicle penetration is increasing due to technical advancements and environmental concerns. Along with residential plug-in electric vehicle charging, the public charging infrastructure is much needed to reduce plug-in electric vehicles' range anxiety and foster their adoption. Renewable energy and demand management programmes are considered viable options that can reduce the impacts of widespread plug-in electric vehicle penetration on the electric grid. This research studies the impacts of plug-in electric vehicle direct current fast charging on a simulated standalone retail building's peak demand and energy consumption, and presents the ability of renewable energy and demand management options to reduce their impacts. Additionally, insights into a public charge station usage are presented by monitoring different types of plug-in electric vehicle charge behaviours at a retail site. Research findings indicate that demand management of building end-use loads along with the use of solar photovoltaic can contribute to absorbing plug-in electric vehicle penetration at the building level ranging from the average of 7% for the demand management option alone to an average of 38% for the combination of demand management and solar photovoltaic, and contributing to shifting building peak demand to late evening hours.

18/00216 Dissipativity based distributed economic model predictive control for residential microgrids with renewable energy generation and battery energy storage

Zhang, X. *et al. Renewable Energy*, 2017, 100, 18–34.

The combination of renewable energy generation and battery energy storage has been widely recognized as a promising solution to the problems associated with variability of renewable energy in residential microgrid. However, due to the low renewable feed-in tariffs in many countries, microgrid users are generally not motivated to install expensive battery systems if they can only be used to satisfy the objective of grid operator. From this perspective, a microgrid power market that encourages users to install batteries for energy-trading will be helpful for the deployment of batteries. For such circumstances, this paper introduces a user-driven microgrid power market. The possible pricing schemes are discussed and an illustrative price controller is presented. The potential destabilizing effect of the collective trading behaviour of users is analysed. A novel dissipativity based distributed economic model prediction control approach is proposed to allow microgrid users to optimize their own benefits while ensuring the performance and stability of the residential microgrid. A simulation study with photovoltaic energy generation and vanadium redox batteries is presented to illustrate the efficacy of the proposed method.

18/00217 Economic, welfare and environmental impact of feed-in tariff policy: a case study in Iran

Tabatabaei, S. M. *et al. Energy Policy*, 2017, 102, 164–169.

Following a particular attention given to environmental issues over the last few decades, establishing proper developmental policies to increase electricity production from renewable energy (RE) has not only been an important issue but also a challenge for many countries. Feed-in tariff (FIT) policy is one of the tools that is being used to facilitate the development of RE. This research evaluated the economic, welfare and environmental impact of this policy on Iran's economy. Therefore, after developing an economic–energy–environmental (E3) type of hybrid general equilibrium model, the effect of FIT policy was examined under different scenarios in order to find an optimal condition in which 10% of electrical energy could be produced from renewable resources. The comparison between the results showed that the application of subsidies to RE and the way the government finances these subsidies can affect the results of FIT policy. Meanwhile, regardless of the role considered for the impact of environmental factors, the policies under the scenario of technology neutral is the most efficient, as it has less impact on the decline of GDP of different sectors and also has less financial cost for government.

18/00218 Electrical energy demand efficiency efforts in Brazil, past, lessons learned, present and future: a critical review

Zurn, H. H. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 1081–1086.

Brazil's predominant hydroelectric power production has to be increasingly complemented by thermal generation to face rapid demand growth, slow new hydro plants planning and construction, proportional reduction of possible energy stored in the reservoirs and longer drought periods. The larger the thermal electricity share, the more expensive is the production cost and environmental impact due to fossil fuels. To counter this, new renewable sources such as wind plants are being massively built in addition to more effective measures of energy conservation, based on traditional methods such as the National Program for Electrical Energy Conservation (PROCEL) and peak load tariff differentials, which affect large consumers and is expected to be applied to residential consumers with new digital energy meters. In addition, there is the traditional summer time offset of one hour in higher southern latitude parts of Brazil. The effects of energy savings and peak load reduction are studied in view of optimal power dispatch reasoning, both considering an uncrowded and a potentially congested transmission network where the predominant power production is hydroelectric. Efforts to increase energy savings and efficiency in Brazil are critically analysed at the end of this paper.

18/00219 Electricity consumption and metropolitan economic performance in Guangzhou: 1950–2013

He, Y. *et al. Energy Economics*, 2017, 63, 154–160.

This study analyses the relationship between electricity consumption and metropolitan economic growth for Guangzhou, China using 64 years of annual-frequency data. The capital stock is used as a control variable because of its role in mediating the relationship between energy utilization and economic output. Empirical results indicate unidirectional Granger causality from electricity consumption to metropolitan economic performance in the short run. This is consistent with the argument that dependable electricity infrastructure and service can play a vital role in facilitating economic growth. Implications for conservation efforts and regional development are discussed.

18/00220 Energy consumption transition through the use of electricity for lighting and cooking: evidence from Bhutan

Rahut, D. B. *et al. Renewable Energy Focus*, 2017, 18, 11–21.

Energy ladder hypothesis states that with an increase in income and awareness households gradually switch from biomass to kerosene and finally to ultra-clean, renewable, green energy sources such as electricity. Electricity lies at the top of the energy ladder hypothesis for household energy use. Empirical results support the fact that income, wealth, gender and the educational status of households often influence the switch from dirty to clean energy; however, in some cases, households even with higher incomes, wealth, and education levels use electricity only for lighting but not for both lighting and cooking. This creates a ladder within the energy ladder. Using a nationally representative dataset collected by the government for the Bhutan Living Standard Measurement Study (2003, 2007 and 2012), covering more than 22,000 households, this study examines the factors influencing the use of electricity for lighting, and lighting and cooking by Bhutanese households. The results of multinomial logit model estimation demonstrate that demographic features, wealth and the education levels of households, in addition to access to infrastructure significantly influence a household's use of electricity for lighting and cooking, which supports a ladder within the energy ladder hypothesis.

18/00221 Energy network dispatch optimization under emergency of local energy shortage with web tool for automatic large group decision-making

Liu, X. *Energy*, 2017, 120, 740–750.

By large group decision-making, obtaining large group response plans within a limited amount of time plays a crucial role under emergency of local energy shortage. An energy network dispatch optimization under emergency of local energy shortage has been found to possess broad applications in energy system; however, the existing mechanism did not consider and failed to provide an approach to deal with the large group decision makers taking part in the energy network dispatch optimization. In this paper, the main contribution is that an energy network dispatch optimization under emergency of local energy shortage with web tool for automatic large group decision-making is proposed, in which anytime and anywhere, each expert can login in the system and provide his/her personal preference to the emergency of local energy shortage alternatives, and then the large group response plans to emergency of local energy shortage will be obtained within a limited amount of time. A case study and simulation results are presented that prove that the proposed model is feasible, and achieves better performance of energy network dispatch optimization under emergency of local energy shortage than the method proposed in the literature.

18/00222 Environmental policy design, innovation and efficiency gains in electricity generation

Johnstone, N. *et al. Energy Economics*, 2017, 63, 106–115.

This paper explores the relationship between environmental regulation, innovation, and competitiveness using environmental patent data. The analysis is conducted in two stages. First, a non-parametric frontier analysis is implemented to estimate efficiency scores, including a measure of technological innovation based on patent stocks. Second,

econometric methods are applied to analyse the role of policy stringency and policy design on efficiency. The estimation sample covers thermal power plant sectors in 20 countries from 1990 to 2009. The results show that the stringency of environmental regulations is a significant determinant of productive efficiency with respect to pollutant emissions as well as fuel use. However, these effects turn negative once the level of stringency leaps over a certain threshold. In addition, the paper concludes that the positive effect of regulatory stringency can be diminished by a negative effect of regulatory differentiation with measures which vary in stringency across plant size and age having negative consequences, and these effects are increasing over time. Finally, it is found that integrated approaches to environmental innovation are more likely to bring about efficiency improvements than end-of-pipe technologies.

18/00223 Evaluating ecosystem service trade-offs with wind electricity production in Switzerland

Egli, T. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 863–875.

In Switzerland, different types of land use, including electricity production, compete directly for little available space. The Swiss energy strategy relies heavily on incorporating renewable sources of electricity, including wind. In order to ensure long term efficient, socially acceptable and sustainable electricity production, land-use conflicts should be addressed and properly managed through a comprehensive and balanced process. The authors propose a method to apply the ecosystem service (ES) approach combined with an optimization tool to tackle the complex problems posed by wind electricity development in a topographically challenging landscape. Marxan was used as optimization software to evaluate, assess, and quantify the trade-offs between ES provisioning and wind electricity production. Expressing different ES in comparable units and evaluating the costs to the system when these are lost versus the benefits gained from wind electricity production generated an output of possible solutions. When compared to similar studies modelling wind electricity output that avoid negative interaction with ES throughout Switzerland, the current results using the optimization tool Marxan suggest a solution requiring 13.5% fewer turbines (1903 in an average solution) in order to produce 12 TWh/yr of wind generated electricity and 18% fewer turbines (842 on average) to produce 5 TWh/yr. Thus, using optimization software can lead to more efficient spatial planning solutions. This methodology can be applied toward cost-effective renewable energy development that minimizes opportunity cost in terms of foregone ES provisioning.

18/00224 Impact assessment of electric vehicles on islands grids: a case study for Tenerife (Spain)

Colmenar-Santos, A. *et al. Energy*, 2017, 120, 385–396.

The penetration of electric vehicles is a key instrument in the operation of smart grids. Their active participation in the electrical system is proposed as a tool to increase security of supply, successfully reducing the large differences that occur between periods of higher and lower electricity demand. This research presents an analysis of the vehicle-to-grid impact in low capacity electrical systems, as in the case of islands, aiming to establish a charge/discharge pattern that facilitates the penetration of electric vehicles in weak grids. In such a way, a comprehensive scenario needs to be assessed in order to obtain significant results to be applied not only in islands and outermost regions but also in scaled systems such as mini grids. To achieve this objective, a theoretical method for the efficient charge/discharge management of electric vehicles is proposed, defined by a multi-objective model based on criteria of mobility and technical requirements. The proposed model is applied to the island of Tenerife, which quantifies the electric vehicle penetration in a real case. The results show that grids in islands can assimilate 'low' or 'transition' penetrations of electric vehicles, so their use as storage systems allow to significantly reduce the amplitude difference between valleys and peaks of the electric energy demand curve and thereby to contribute to the efficient management of smart grids.

18/00225 Measuring the progress and impacts of decarbonising British electricity

Staffell, I. *Energy Policy*, 2017, 102, 463–475.

Britain's ambitious carbon targets require that electricity be immediately and aggressively decarbonized, so it is reassuring to report that electricity sector emissions have fallen 46% in the 3 years to June 2016, their lowest since 1960. This paper analyses the factors behind this fall and the impacts they are having. The main drivers are: demand falling 1.3% per year due to efficiency gains and mild winters; gas doubling its share to 60% of fossil generation due to the carbon price floor; and the dramatic uptake of wind, solar and biomass which now supply up to 45% of demand. Accounting conventions also play their part: imported electricity and biomass would add 5% and 2% to emissions if they were included. The pace of decarbonization is impressive, but raises both engineering and economic challenges. Falling peak demand has delayed fears of capacity shortage, but minimum net demand is instead becoming a problem. The headroom between inflexible nuclear and intermittent renewables is rapidly shrinking, with controllable output reaching a minimum of just 5.9 GW as solar output peaked at 7.1 GW. The year 2015 also saw Britain's first negative power prices, the highest winter peak prices for six years, and the highest balancing costs.

18/00226 $NiCo_2O_4$ decorated PANI–CNTs composites as supercapacitive electrode materials

Chaudhary, G. *et al. Journal of Energy Chemistry*, 2017, 26, (1), 175–181.

Hierarchical $NiCo_2O_4$/PANI/CNTs hybrid composites were designed and fabricated having a layer of $NiCo_2O_4$ on the surface of PANI encapsulated CNTs with different morphologies. Physicochemical attributes of the synthesized composites were examined by FTIR, UV-visible and X-ray diffraction techniques. Morphological aspects were evaluated by field-emission scanning microscopy, electron diffraction spectroscopy, high resolution transmission electron microscopy and selected area electron diffraction studies. Electrochemical measurements revealed an improved specific capacitance of 2250 F/g at a scan rate of 5 mV/s and 2000 F/g at a current density of 1 A/g with good rate capability using a three-electrode system. These enhanced features are achieved from the well-designed nanostructure and the synergistic contributions of individual components in the electrode material.

18/00227 Performance assessment of hybrid power generation systems: economic and environmental impacts

Al-Sharafi, A. *et al. Energy Conversion and Management*, 2017, 132, 418–431.

This article aims to introduce a double-step performance assessment tool for the hybrid power generation systems. As a case study, a hybrid system comprising photovoltaic array, wind-turbine, battery bank and diesel engine is incorporated in hourly based simulations to meet power demand of a residence unit at Dhahran area, Saudi Arabia. Different indicators related to economic and environmental performance assessments of the hybrid system have been considered. In the economic related assessment case, cost of electricity, energy excess percentage, and operating life cycle indicators have been considered and combined to develop the first overall performance index. Renewable contribution, renewable source availability and environmental impact indicators have been considered for the environmental assessment case and they are combined in the second performance index. For either economical or environmental cases, the optimum configuration of the system is achieved by maximizing the first and second overall performance indicators. This innovative optimization tools gives the designer the freedom to assign suitable weights associated with economical aspect, environmental impact, governmental regulations and social impact, for the first and second overall performance indicators, and combine them in the total performance index. The optimum system configuration is at the point where the total performance index is maximized.

18/00228 Risk assessment of dynamic system cascading collapse for determining the sensitive transmission lines and severity of total loading conditions

Salim, N. A. *et al. Reliability Engineering & System Safety*, 2017, 157, 113–128.

This paper presents a computationally accurate technique used to determine the estimated average probability of a dynamic system cascading collapse considering the effect of hidden failure on a protection system. This requires an accurate calculation of the probability of hidden failure as it will give significant effect on the results of the estimated average probability of dynamic system cascading collapse. The estimated average probability of a dynamic system cascading collapse is then used to determine the severe loading condition contributing to a higher risk of a system cascading collapse. This information of risk assessment is important to the utility that will assist them to determine the maximum level of increase in the system loading condition before a critical dynamic system cascading collapse is incurred. Furthermore, initial tripping of sensitive transmission line contributing to a dynamic critical system cascading collapse can also be determined by using the proposed risk assessment. Based on the results obtained from this study, it was found that selecting the accurate probability of hidden failure is very important as it will affect the estimated average probability of a dynamic system cascading collapse used for determining the results of sensitive transmission lines and severity of total loading conditions.

18/00229 Strategic capacity withholding through failures in the German-Austrian electricity market

Bergler, J. *et al. Energy Policy*, 2017, 102, 210–221.

In electricity day-ahead markets organized as uniform price auction, a small reduction in supply in times of high demand can cause substantial increases in price. The authors use a unique data set of failures of

generation capacity in the German–Austrian electricity market to investigate the relationship between electricity spot prices and generation failures. Differentiating between strategic and non-strategic failures, a positive impact of prices on non-usable marginal generation capacity was found for strategic failures only. This empirical analysis therefore provides evidence for the existence of strategic capacity withholding through failures suggesting further monitoring efforts by public authorities to effectively reduce the likelihood of such abuses of a dominant position.

18/00230 Testing for convergence in electricity consumption across Croatian regions at the consumer's sectoral level
Borozan, D. *Energy Policy*, 2017, 102, 145–153.
Using the panel unit tests with and without structural break(s), the convergence hypothesis in relative per capita electricity consumption series is tested across Croatian regions during the period 2001–2013. The results are mixed, depending primarily on the consumption sector considered and the test applied. They indicate the necessity to conduct analysis and formulate energy policy measures on the sector-disaggregated and regional-specific electricity consumption time series. The Croatian electricity markets are not fully integrated, and some regions are faced with statistically significant structural break(s), demonstrating thereby the Croatian gradual energy reform process with several sudden innovations, significant regional differences, and the market dependence on expectations, domestic and international economic and non-economic innovations. The impacts of innovations are likely to be permanent for most of the regions, and their electricity consumption behaviours are likely to be path dependent. Consequently, innovations into the energy markets, including government interventions, may have long-run effects, indicating that space and time for experimenting with alternative mechanisms are quite limited.

18/00231 The 'German Paradox' in the balancing power markets
Ocker, F. and Ehrhart, K.-M. *Renewable and Sustainable Energy Reviews*, 2017, 67, 892–898.
This paper provides answers to questions raised in an earlier paper regarding the 'German paradox; in the balancing power markets. The authors show that in spite of the increasing energy production from variable renewable energy sources, there is no need for a higher demand of balancing power in Germany because adaptations in the energy market design were undertaken and grid control cooperation led to immense efficiency savings. Additionally, they investigate the price developments in the German Secondary balancing power market. Evidence was found that the suppliers coordinate on a price level which is (far) above the competitive level and that they orientate their power bids towards previous auction prices.

18/00232 The real options to shutdown, startup, and abandon: U.S. electricity industry evidence
Fleten, S.-E. *et al. Energy Economics*, 2017, 63, 1–12.
The purpose of this paper is to examine empirically the partially irreversible decisions to shutdown, start-up and abandon existing production assets under cash flow uncertainty and regulatory uncertainty. The authors use detailed information for 1121 individual electric power generators located in the USA for the period 2001–2009 and find strong evidence of real options effects. It was found that both profitability uncertainty and regulatory uncertainty decrease the probability of shutdown. Regulatory uncertainty also decreases the probability of start-up, but it was found that cash flow uncertainty increases the probability of start-up, especially for large generators.

18/00233 Wind farms participation in electricity markets considering uncertainties
Dehghani, H. *et al. Renewable Energy*, 2017, 101, 907–918.
Rising global temperature and environmental pollution as well as the demand for energy consumption have made finding new and affordable clean energy resources a serious challenge for governments. A possible solution could be renewable resources such as solar, wind or geothermal energies. Restructuring and deregulation have provided a competitive environment which makes analysis of these new energy sources necessary. Wind farms have been receiving more attention from governments because of their noticeable generation capability. The stochastic nature of the wind inflicts uncertainty on the output generation of wind farms which then causes some limitations for the participation of these farms in the electricity market. Thus, in this paper the effects of uncertainty in predicting the wind farm's power on locational marginal price in the market have been studied. According to the advantages and disadvantages of wind farm's power uncertainties, a procedure to maximize the social welfare is presented. The studies have been done on an 8-bus network for 24 h in a day-ahead electricity market. To do this, the farm power is predicted using neural network and wavelet transform and its uncertainties are calculated using the asymmetric Quantile Regression method.

07 STEAM RAISING

Boiler operation/design

18/00234 A modeling approach to co-firing biomass/coal blends in pulverized coal utility boilers: synergistic effects and emissions profiles
Pérez-Jeldres, R. *et al. Energy*, 2017, 120, 663–674.
Pulverized coal power plants in Chile are evaluating to reduce CO_2 emissions by co-firing coal with biomass, which is CO_2-neutral. A computational fluid dynamics model was used in this study to predict the performance of a 150 MW commercial boiler co-firing pulverized coal with pine sawdust. Synergistic effects were identified by burnout, thermal and hydrodynamic profiles. Co-firing was simulated with 5% of biomass substitution, and feeding in the first level of burners. The model was validated using data from the power plant. The results show an expected decrease in SO_2 emissions and a negligible reduction in heat transferred to the water tubes (0.6%). Biomass presence increased the burning rate of fuel particles, as shown by higher CO_2 emissions and a lower CO concentration, per unit of thermal power. The model reveals synergistic effects, proved by an increase in temperature, due to an early combustion of biomass particles, increase in the coal combustion rate, and a better temperature distribution in the boiler. These synergistic effects were compared with results obtained at bench scale reported in the literature. Thus, it was concluded that a relatively small replacement of coal by biomass could significantly improve the fuel combustion process and the boiler performance.

18/00235 Mathematical model for integrated coal fired thermal boiler using physical laws
Sreepradha, C. *et al. Energy*, 2017, 118, 985–998.
The boiler of coal-fired thermal power plant consists of integrating process units such as the furnace, economizer, drum, and superheater. There is a lack of proper dynamic model derived from mass and energy balances of individual units integrated together where dynamics of material and energy flow are not understood properly supporting the larger footprints and environmental impact of the specific industry. This paper considers formulation of simple mathematical models for integrated boiler units based on first principle laws (excluding furnace). The derived equations are validated with the real-time plant data from 210 MW coal-fired thermal power plant. Though temperature and pressures are convertible at equilibrium through Clausius–Clapeyron equation, the model supports for level, temperature and pressure measurements and predictions. The effects of change in parameters of the boiler are studied and discussed in detail. The model can be used for further process control studies.

18/00236 Performance comparison of SOFC integrated combined power systems with three different bottoming steam turbine cycles
Sarmah, P. and Gogoi, T. K. *Energy Conversion and Management*, 2017, 132, 91–101.
In this article, a thermodynamic model is developed for analysing the energetic and exergetic performance of a solid oxide fuel cell (SOFC) integrated combined power system with triple pressure reheat cycle in the bottoming steam turbine (ST) plant. A temperature difference range of 15–20 °C is considered between flue gas and steam at superheater inlet in the high and intermediate pressure stages of the heat recovery steam generator (HRSG). Also, a temperature difference of 20 °C is maintained at the pinch point between flue gas and saturated water in the low pressure stage of the HRSG. Detail performance variation is provided as a function of compressor pressure ratio (CPR) showing that the system's power and efficiency increase while total irreversibility decreases at higher CPR. Further, thermodynamic modelling is done for two other systems with dual pressure reheat and single pressure ST cycles for performance comparison amongst all, under identical conditions. The comparative study shows that the system with single pressure ST cycle performs better compared to the others; the highest power is obtained from this system with minimum total irreversibility. It is recommended that the system with single pressure ST cycle would be the most appropriate as it is simple with less number of components and minimum total cost.

18/00237 Steam gasification of biomass with subsequent syngas adjustment using shift reaction for syngas production: an Aspen Plus model
Pala, L. P. R. *et al. Renewable Energy*, 2017, 101, 484–492.
A simulation model of biomass gasification for syngas production with steam as gasifying agent and subsequent syngas adjustment has been developed using Aspen Plus. The developed model is based on Gibbs

free energy minimization applying the restricted equilibrium method. The objective is to study the effect of important parameters such as gasification temperature, steam to biomass ratio and shift reaction temperature on hydrogen concentration, CO concentration, CO conversion, CO_2 conversion and H_2/CO ratio in the syngas. Simulations were performed for different biomass feedstocks to predict their syngas composition. The hydrogen and CO concentrations were altered such that the H_2/CO molar ratio in the syngas composition gets adjusted close to a value of 2.15 as required for FT synthesis by the shift reaction. The present model has been validated with experimental data from literature on steam biomass gasification conducted in a research scale fluidized bed gasifier. The product gas obtained from steam gasification of food wastes resulted in a composition with a H_2/CO molar ratio close to 2.15 which can be directly fed to a Fischer–Tropsch synthesis plant whereas remaining feedstocks requires a syngas adjustment either by WGS or RWGS reactions to achieve H_2/CO molar ratio close to 2.15.

18/00238 Wellbore modeling for hybrid steam-solvent processes

de Almeida, R. V. *et al. Fuel*, 2017, 188, 50–60.

The addition of hydrocarbon solvents to the cyclic steam stimulation (CSS) or steam assisted gravity drainage (SAGD) processes has recently gained significant interest from the petroleum industry. In these processes, a proper selection of solvent is critical: injected solvent must be in the vapour phase at the injection point in order to propagate inside the steam chamber and condense at the steam/oil interface to effectively reduce oil viscosity. Therefore, the wellbore have to deliver vaporized solvent near its dew point at perforation intervals. This work provides a detailed numerical formulation to predict steam and solvent qualities, temperature, and pressure profiles along the wellbore. Four phases were considered: hydrocarbon liquid and vapour phases, and aqueous liquid and vapour phases. The mass, energy and momentum balance equations are integrated with drift-flux model and discretized over the wellbore domain. Unknowns and governing equations are divided into the sets of primary and secondary equation and unknowns are solved sequentially. The model was compared against previously published models and field data. The data from two steam injection wells and two gas condensate production wells were used for validation. Also, case studies are presented to investigate the temperature and condensation behaviour of the solvent-steam mixture. The use of this model will assist the industry in proper wellbore design and the engineering of injection constraints in hybrid steam/solvent injection processes.

08 COMBUSTION

Burners, combustion systems

18/00239 A comprehensive study on pyrolysis kinetics of microalgal biomass

Bach, Q.-V. and Chen, W.-H. *Energy Conversion and Management*, 2017, 131, 109–116.

Pyrolysis of microalgal biomass for biofuels production has attracted much attention. However, detailed degradation mechanism and kinetics of the process have not been fully explored yet. In this study, a non-isothermal pyrolysis of microalga *Chlorella vulgaris* ESP-31 is thermogravimetrically investigated. Several kinetic models, from a single reaction to seven parallel reactions, are tested to fit the experimental pyrolysis data for finding out the optimal pyrolysis model. The results show that the pyrolysis behaviour of the microalga is somewhat different from that of lignocellulosic biomass, stemming from the inherent difference in their compositions. Overall, the kinetic modelling processes show that increasing the number of reactions improves the model fit quality. Curve fitting results indicate that the models consisting of three and less than three reactions are not suitable for microalga pyrolysis. The four-reaction model, via considering the pyrolysis of carbohydrate, protein, lipid and others, can be employed for modelling the thermal degradation; however, it cannot precisely predict the thermal degradation of the shoulder and the small peak. The conducted seven-reaction model further partitions the decomposition processes of carbohydrate and protein into two stages, and explains the thermal degradation well. The model indicates that the devolatilization peak is attributed to the combined degradation of protein I and carbohydrate II. The seven-reaction model offers the highest fit quality and is thus recommended for predicting the microalga pyrolysis processes.

18/00240 A novel gel combustion procedure for the preparation of foam and porous pellets of UO_2

Kumar, D. S. *et al. Journal of Nuclear Materials*, 2017, 483, 199–204.

In this study, it has been demonstrated for the first time how sucrose gel-combustion could be used for the preparation of UO_2 foam. Further the citrate gel-combustion was gainfully used for preparing porous pellets of UO_2. The utility of two-step sintering (1073 K for 30 min and 1473 K for 4 h) for obtaining these porous bodies was demonstrated for the first time. The foams and pellets possessed meso and macro pores. A starting mixture with sucrose to nitrate ratio of 2.4 was found to yield urania foam with adequate crush strength. The porous pellets were found to possess better handling strength, lesser carbon residue and higher overall density than the foam. A citric acid to nitrate ratio 0.25 in the starting mixture, 180 MPa compaction pressure were optimal for obtaining a pellet with 40% porosity.

18/00241 Comparative pyrolysis behaviors and reaction mechanisms of hardwood and softwood

Ding, Y. *et al. Energy Conversion and Management*, 2017, 132, 102–109.

Comparative pyrolysis behaviours of a typical hardwood (*Fagus sylvatica*) and softwood (*Cunninghamia lanceolata*) were investigated based on thermogravimetric analysis over a wide heating rate range from 5 to 60 K/min. The Flynn–Wall–Ozawa model-free method was applied to estimate the various activation energy values at different conversion rates, and the Coats–Redfern model-fitting method was used to predict the possible reaction mechanism. Two pyrolysis regions were established by the trend of activation energy, divided by the threshold of conversion rate (0.4 for hardwood and 0.2 for softwood) but with the same distinguished temperature at about 580 K. For the region under the conversion rate threshold, the activation energy of hardwood increased gradually while softwood decreased. Furthermore, the activation energy remained the same for both hardwood and softwood in the region over the conversion rate threshold. However, softwood behaved greater activation energy than hardwood during the whole pyrolysis process. The pyrolysis differences of hardwood and softwood could be attributed to the chemical component, molecular structure, component proportion and various extractives. The same reaction mechanism of hardwood and softwood was verified by applying the Coats-Redfern approach. By checking activation energies obtained according to different models with those obtained through the Flynn-Wall-Ozawa method, the best model was based on diffusion mechanism when the conversion rate was less than its threshold, otherwise based on reaction order (second to third).

18/00242 High oxidation activity of thallium oxide for carbon combustion

Nakayama, S. and Sakamoto, M. *Thermochimica Acta*, 2017, 647, 81–85.

The catalytic behaviour of thallium(III) oxide (Tl_2O_3) with respect to the combustion of carbon black was investigated using thermal analysis, X-ray diffraction analysis, scanning electron microscopy, and the ^{18}O-isotope exchange technique. The thermogravimetric-differential thermal analysis results revealed that the combustion temperature of carbon black (650 °C) decreases dramatically, to 320 °C, when it is mixed with Tl_2O_3 (2 wt% carbon black + as-purchased Tl_2O_3), owing to its oxidation by Tl_2O_3, which has the ability to readily release its lattice oxygens.

18/00243 Infrared laser-absorption sensing for combustion gases

Goldenstein, C. S. *et al. Progress in Energy and Combustion Science*, 2017, 60, 132–176.

Infrared laser-absorption spectroscopy (IR-LAS) sensors play an important role in diagnosing and characterizing a wide range of combustion systems. Of all the laser-diagnostic techniques, LAS is arguably the most versatile and quantitative, as it has been used extensively to provide quantitative, species-specific measurements of gas temperature, pressure, composition and velocity in both laboratory- and industrial-scale systems. Historically, most IR-LAS work has been conducted using tuneable diode lasers; however, today's researchers have access to a wide range of light sources that provide unique sensing capabilities and convenient access to nearly the entire IR spectrum (≈0.8–16 μm). In particular, the advent of room-temperature wavelength-tuneable mid-infrared semiconductor lasers (e.g. interband- and quantum-cascade lasers) and hyperspectral light sources (e.g. MEMS VCSELs, Fourier-domain mode-locked lasers, dispersed supercontinuum, and frequency combs) has provided a number of unique capabilities that combustion researchers have exploited. The primary goals of this review paper are: (1) to document the recent development, application, and current capabilities of IR-LAS sensors for laboratory- and industrial-scale combustors and propulsion systems, (2) to elucidate the design and use of IR-LAS sensors for combustion gases through a discussion of the modern sensor-design process and state-of-the-art techniques, and (3) to highlight some of the remaining measurement opportunities, challenges, and needs. A thorough review

and description of the fundamental spectroscopy governing the accuracy of such sensors, and recent findings and databases that enable improved modelling of molecular absorption spectra will also be provided.

18/00244 LES of pulverized coal combustion with a multi-regime flamelet model

Wen, X. *et al. Fuel*, 2017, 188, 661–671.

It is well known that premixed and non-premixed flamelets coexist in the combustion system, especially for multiphase combustion. In this work, a multi-regime combustion model for partially premixed multiphase combustion (2PMC) is developed in the framework of large eddy simulation (LES). In this model, the multi-regime combustion mode is decomposed into two pure combustion regimes (i.e. premixed and non-premixed) through combustion regime indicator. Different combustion models are chosen for different combustion regimes. For example, for premixed combustion regime, the flamelet generated manifold (FGM) tabulation method in combination with the artificially thickened flame (ATF) approach is used. For non-premixed combustion regime, on the other hand, the thermo-chemical quantities will be extracted from the non-premixed chemtable generated by the flamelet/progress variable (FPV) approach. The proposed multi-regime flamelet model is then extended to adapt to the pulverized coal combustion (PCC) and applied to a laboratory-scale pulverized coal jet flame. The simulation results show that the percentage of the volume-weighted premixed combustion regime of this studied flame is up to 18%. Quantitative comparisons between the experimental data and the numerical results with the present multi-regime flamelet model, the FPV model, and the eddy break up (EBU) model shows that the proposed multi-regime flamelet model has several advantages. It performs better than the FPV model in the regions where premixed combustion mode prevails and also much better than the EBU model in species concentration prediction.

18/00245 Nanosized zero-valent iron as Fenton-like reagent for ultrasonic-assisted leaching of zinc from blast furnace sludge

Mikhailov, I. *et al. Journal of Hazardous Materials*, 2017, 321, 557–565.

Ultrasonic-assisted sulfuric acid leaching combined with a Fenton-like process, utilizing nanoscale zero-valent iron (nZVI), was investigated to enhance the leaching of zinc from the blast furnace sludge (BFS). The leaching of iron (Fe) and zinc (Zn) from the sludge was investigated using Milli-Q water/BFS ratio of 10 and varying the concentration of hydrogen peroxide, sulfuric acid, the temperature, the input energy for ultrasound irradiation, and the presence or absence of nZVI as a Fenton reagent. The results showed that with 1 g/l addition of nZVI and 0.05 M of hydrogen peroxide, the kinetic rate of Zn leaching increased with a maximum dissolution degree of 80.2%, after 5 min treatment. In the absence of nZVI, the maximum dissolution degree of Zn was 99.2%, after 15 min treatment with 0.1 M of hydrogen peroxide. The rate of Zn leaching at several concentrations of hydrogen peroxide is accelerated in the presence of nZVI although a reduction in efficiency was observed. The loss of Fe was no more than 3%. On the basis of these results, the possible route for BFS recycling has been proposed (BFS slurry mixed with sulfuric acid and hydrogen peroxide is recirculated under ultrasonic irradiation then separated).

18/00246 Numerical modelling of soot formation and oxidation using phenomenological soot modelling approach in a dual-fueled compression ignition engine

Zhao, F. *et al. Fuel*, 2017, 188, 382–389.

Modelling soot formation and oxidation in diesel engines has been a long-standing challenge. In this study, soot particle characteristics in terms of particle dynamics, particle size and number density were modelled by integrating a multi-step phenomenological soot model into the KIVA-CHEMKIN CFD code for compression ignition engine combustion simulations. This semi-detailed soot model is dedicated to solving rate equations using sub-models to account for precursor formation, soot particle inception and coagulation as well as soot surface growth and oxidation. Soot growth and oxidation is inherently derived from the concentration of certain species found in the chemical reaction mechanism used, namely H, O_2, C_2H_2 and the nucleating polycyclic aromatic hydrocarbon (PAH). Acetylene is taken as the core precursor species in nucleating PAH, soot inception as well as acetylene-assisted soot surface growth. The integrated multi-step phenomenological soot model has been validated under gasoline and diesel dual-fuel engine conditions. The predicted histograms of soot particle number along with size distribution contribute towards the understanding of dominant factors that affect soot formation. The factors affecting soot particle under varying engine loads and fuel conditions were extensively investigated. Generally, the predicted soot particle size was larger for heavy-sooting conditions as compared to low-sooting conditions. For port-injected gasoline-dominated combustion, there is less soot being discharged. This might be attributed to two reasons. First, a more homogenous mixture is realized with less diesel fuel, thus effectively reducing the formation of soot precursors. The other reason is the intensive heat release which enhances the depletion of soot precursors, thereby impeding the growth of soot particles in terms of size and mass.

18/00247 On the oxy-combustion of lignite and corn stover in a lab-scale fluidized bed reactor

Lupiá, C. *et al. Biomass and Bioenergy*, 2017, 96, 152–161.

This paper addresses an experimental investigation concerning oxy-combustion of coal and biomass in a lab-scale fluidized bed reactor. While co-firing has been widely studied under conventional air conditions, few experiences are available to date for O_2/CO_2 atmospheres. The research is focused on SO_2 and NO_x emissions, along with the deposition rates and ashes mineralogy. The influences of the atmosphere (air vs 30/70% O_2/CO_2), the coal-to-biomass energy input ratio (80/20%, 90/10%), the chlorine mass fraction in the biomass (0.35%, 1%, 2%) and the Ca : S mole ratio (2.5, 4) are reported and discussed in the paper, for two specific fuels: high sulfur lignite and high chlorine corn stover. Concerning SO_2 emissions a correlation among the sulfur and the chlorine contents is clearly detected, being affected by the direct desulfurization mechanism occurring under oxy-firing conditions. The single effect of the chlorine content is found to be almost 1.5% of the desulfurization efficiency. NO_x emissions are otherwise more dependent on oxygen excess and CO concentration in the reactor, rather than the fuel share or the chlorine supplied. Thick deposition is only detected when chlorine content in the corn is 2%. Potassium aluminosilication is found to be enhanced in comparison to potassium sulfation under oxy-firing, especially for the highest Ca : S mole ratio: observed aluminosilication is five times higher when Ca : S ratio is increased from 2.5 to 4. A significant enrichment in iron is also detected for the fly ash composition, with an increase of 30–50% in comparison to air combustion.

18/00248 Potential pyrolysis pathway assessment for microalgae-based aviation fuel based on energy conversion efficiency and life cycle

Guo, F. *et al. Energy Conversion and Management*, 2017, 132, 272–280.

Although the research of microalgae pyrolysis has been conducted for many years, there is a lack of investigations on energy efficiency and life cycle assessment. This study investigated the biocrude yield and energy efficiency of direct pyrolysis, microalgae residue pyrolysis after lipid extraction (indirect pyrolysis), and different microalgae co-pyrolysis. This research also investigated the life cycle assessment of the three different pyrolysis pathways. A system boundary of well-to-wake (WTWa) was defined and included sub-process models, such as feedstock production, fuel production and pump-to-wheels (PTW) stages. The pathway of *Isochrysis* indirect pyrolysis shows the best performance in the mass ratio and energy ratio, produces the most kerosene component precursor, has the lowest WTWa total energy input, fossil fuel consumption and greenhouse gas emissions, and results in the best energy efficiency. All the evidence indicates that *Isochrysis* R2 pathway is a potential and optimal pyrolysis pathway to liquid biofuels. The mass ratio of pyrolysis biocrude is shown to be the decisive factor for different microalgae species. The sensitivity analysis results also indicates that the life cycle indicators are particularly sensitive to the mass ratio of pyrolysis biocrude for microalgae-based hydrotreated pyrolysis aviation fuel.

18/00249 Pyrolysis of pellets made with biomass and glycerol: kinetic analysis and evolved gas analysis

Bartocci, P. *et al. Biomass and Bioenergy*, 2017, 97, 11–19.

Glycerol is a co-product compound of biodiesel production with an interesting heating value. In this work pyrolysis kinetic parameters for a pellet made with a mass fraction of 90% sawdust and a mass fraction of 10% glycerol are derived through thermogravimetric analysis. A new parallel reaction scheme with four components (cellulose, hemicellulose, lignin and glycerol) is adopted and the kinetic triplet for each component is derived using a model fitting approach applied to this particular kind of pellet. The isoconversional method of Kissinger–Akahira–Sunose is employed both to provide initial values for model fitting simulations and to check final results. Results show that activation energies and pre-exponential factors are respectively: 149.7 kJ mol^{-1} and 1.98×10^{11} s^{-1} for hemicellulose, 230.1 kJ mol^{-1} and 1.84×10^{17} s^{-1} for cellulose, 154.3 kJ mol^{-1} and 5.14×10^{9} s^{-1} for lignin, 74.5 kJ mol^{-1} and 2.17×10^{5} s^{-1} for glycerol with a first reaction order for all components, except for lignin ($n = 2.6$). Through evolved gas analysis it was demonstrated that the thermal degradation of glycerol contained in the pellet can increase hydrogen content in pyrolysis gases.

18/00250 Shock tube study of *n*-nonane/air ignition over a wide range of temperatures

Yong, K. *et al. Fuel*, 2017, 188, 567–574.

Ignition delay experiments for gas phase *n*-nonane/air mixtures have been performed behind reflected shock waves over a wide temperature range of 684–1448 K, pressures of 2.0–15.0 atm, and equivalence ratios of 0.5, 1.0 and 2.0. Ignition delay times were determined using electronically excited CH emission and reflected shock pressure signals monitored at the sidewall of the shock tube. A negative-temperature-coefficient (NTC) behaviour of *n*-nonane/air ignition was observed at temperatures of 800–950 K. Dependence of ignition delay time upon temperature, pressure, and equivalence ratio was investigated systematically. High temperature ($T > 1000$ K) results show that the effect of equivalence ratio on ignition delay times is different at low and high pressures. In the NTC region, ignition delay times are highly sensitive to equivalence ratio and pressure. The present ignition data are in satisfactory agreement with predictions of two widely used chemical kinetic mechanisms. Sensitivity and reaction pathway analyses reveal that the dominating reactions affecting ignition delay times and reaction pathways during ignition process for *n*-nonane/air are quite different at high and low temperatures. Comparison of *n*-nonane/air ignition delay times with those of other larger *n*-alkanes (*n*-heptane, *n*-octane, *n*-decane, *n*-dodecane, and *n*-tetradecane) indicates that the length of *n*-alkanes chain influences little on ignition delay times of *n*-alkanes. The present results are useful for understanding ignition characteristics of *n*-nonane and providing experimental data to validate chemical kinetic mechanisms for *n*-nonane.

18/00251 Simultaneous removal of multi-pollutants from flue gas by a vaporized composite absorbent

Zhao, Y. *et al. Journal of Hazardous Materials*, 2017, 321, 500–508.

An economical process that was used to remove SO_2, NO and Hg^0 simultaneously was developed, based on the pre-oxidations of Hg^0 and NO by a vaporized Fenton-based complex oxidant (FO) consisted of Fenton and NaClO. The effects of concentrations of $FeSO_4$ and NaClO in the oxidant, the molar ratio of vaporized oxidant to multi-pollutant, the oxidant solution pH, the reaction temperature, the gas flow ratio of vaporized FO to multi-pollutants, the flue gas flow and the concentrations of coexistence gases in flue gas on the simultaneous removals were investigated experimentally. The results showed that the removals of NO and Hg^0 were significantly depended on $FeSO_4$ and NaClO concentrations, the molar ratio of vaporized oxidant to multi-pollutants, the FO solution pH, the reaction temperature, the gas flow ratio of vaporized FO to multi-pollutants and flue gas flow. And higher concentration of SO_2 and an appropriate concentration of NO had the promotion for Hg^0 removal. The average simultaneous removal efficiencies of 100% for SO_2, 81% for NO and 91% for Hg^0 were obtained under the optimal reaction conditions. According to the characterization of the reaction removal products by SEM, EDS, XRD and AFS, the reaction mechanism was speculated.

Fire safety

18/00252 A new shock factor of SWATH catamaran subjected to underwater explosion

Guo, J. *et al. Ocean Engineering*, 2017, 130, 620–628.

In order to measure the extreme degree of the impact environment on a small waterplane area twin hull (SWATH) catamaran subjected to an underwater explosion, this work defines a new type of shock factor based on shock wave energy. This new shock factor is used as a parameter to describe the response from this kind of ship, and it is divided into two categories according to characteristics of the SWATH catamaran structure. This research used finite element software to simulate and calculate the response of SWATH catamaran subjected to an underwater explosion. The validity of this new shock factor is proved in three categories, including total kinetic energy, total strain energy and shock spectrum. The results show that the responses of the SWATH catamaran structure are similar when the new shock factor is equal, and it is also appropriate for situations involving short explosive distances.

18/00253 An experimental investigation into the effect of substrate slope on the continuously released liquid fuel spill fires

Li, Y. *et al. Journal of Loss Prevention in the Process Industries*, 2017, 45, 203–209.

The spread of burning fuel spilled from tanks or pipes during oil storage and transportation industries may threat other facilities nearby and trigger further accidents. In this paper, the effect of substrate slope on the continuously released liquid fuel spill fire was experimentally investigated, in a one-dimensional channel with different discharge rates and substrate slope angles. The time-varying burning area was recorded and analysed, with five typical phases. It is observed that the maximum burning area increases largely with the increasing slope angle, while the steady burning area increases only a little. The steady burning rate, which equals the ratio of the discharge flow rate to the steady burning area, decreases with the increasing slope angle. It is proved that the burning rate for liquid fuel spill fire is much lower than that of pool fire with the same dimensions. The facilities and data presented in this work may provide a basis for the future modelling study of the liquid fuel spill fire on inclined surface.

18/00254 Determination of design accidental fire load for offshore installations based on quantitative risk assessment with treatment of parametric uncertainty

Chu, B. *et al. Journal of Loss Prevention in the Process Industries*, 2017, 45, 160–172.

This study investigated the critical issues for determining the design accidental load (DAL) fire procedure based on quantitative risk assessment (QRA) for offshore installations. Considerable attention was paid to parametric uncertainty in choosing the numerical values used for the frequency and consequence analysis. In particular, selecting the initial leak size was one of the most critical aspects, and inconsistent approaches for selecting this value resulted in different risks for identical systems. Frequency analysis of past investigations also overlooked the inaccuracy and unsuitability of statistical data. Accordingly, the estimated risks were significantly uncertain, and the lack of information about the results increased the risk of making the wrong decision. In this study, the Latin hypercube sampling (LHS) technique was used to treat parametric uncertainty in QRA. Different fire exceedance curves and DAL fires were demonstrated by selecting different sets of representative values. The distribution and confidence interval of the DAL fires showed a wide distribution with varying uncertain and critical parameters. Therefore, this procedure provided quantitative information on inherent uncertainty, and such additional information regarding DAL fires can lead to better decision making.

18/00255 Experimental study on the flame acceleration of premixed hydrocarbons-hydrogen/air mixtures in tee pipes

Emami, S. D. *et al. Journal of Loss Prevention in the Process Industries*, 2017, 45, 229–241.

The benefits of using hydrogen as a source of fuel seem to be limited due to a number of difficulties. To overcome the drawbacks of hydrogen, hydrocarbon–hydrogen fuel mixtures are the best substitutions. However, in literature, the flame acceleration of hydrogen-hydrocarbons/air mixtures in tee pipes has not yet been fully explored. Thus, the aim of this work is to report some new experimental data and provide an understanding of the explosion development in the geometry of tee pipes. In this study, premixed C_2H_4–H_2/air, NG-H_2/air and C_3H_8–H_2/air mixtures with different ratios of 10 : 90, 30 : 70, 50 : 50, 70 : 30 and 90 : 10 were ignited at six ignition positions at two tee pipe configurations. Hydrocarbon fuels were considered as the primary gases. For the overall observation, it can be said that the flame reactivity of ethylene–hydrogen/air and NG–hydrogen/air was much higher. The kinetic reaction of these mixtures contributed to the overall explosion development. However, the dynamics of flame deployment in the tee junctions had a significant effect on the recorded maximum overpressure and flame speeds along the pipes. Moreover, the obtained data show that the lower distance of tee junction to ignition point caused a higher explosion severity in terms of the rate of pressure rise.

18/00256 External heating of electrical cables and auto-ignition investigation

Courty, L. and Garo, J. P. *Journal of Hazardous Materials*, 2017, 321, 528–536.

Electric cables are now extensively used for both residential and industrial applications. During more than twenty years, multi-scale approaches have been developed to study fire behaviour of such cables that represents a serious challenge. Cables are rather complicated materials because they consist of an insulated part and jacket of polymeric materials. These polymeric materials can have various chemical structures, thicknesses and additives and generally have a char-forming tendency when exposed to heat source. In this work, two test methods are used for the characterization of cable pyrolysis and flammability. The first one permits the investigation of cable pyrolysis. A description of the cable mass loss is obtained, coupling an Arrhenius expression with a 1D thermal model of cables heating. Numerical results are successfully compared with experimental data obtained for two types of cable commonly used in French nuclear power plants. The second one is devoted to ignition investigations (spontaneous or piloted) of these cables. All these basic observations, measurements and modelling efforts are of major interest for a more comprehensive fire resistance evaluation of electric cables.

18/00257 Flame-retardant EPDM compounds containing phenanthrene to enhance radiation resistance

Chen, J. *et al. Radiation Physics and Chemistry*, 2017, 130, 400–405.

Ethylene propylene diene monomer (EPDM) compounds with good flame-retardant and γ-ray radiation resistant properties were prepared by adding complex flame retardants and phenathrene. The resultant EPDM formulations have a long time to ignition (TTI >46 s), a low peak heat release rate (PHRR $\sim$ 341 kW/m^2) and a high limited oxygen index (LOI > 30). Effects of γ-ray radiation on the resultant flame-retardant EPDM was investigated. The formulated EPDM is a crosslinking dominated polymer under γ-ray radiation. The γ-ray radiation resistant property of EPDM was enhanced by adding phenanthrene. Elongation at break of EPDM formulated with phenanthrene could retain 91% after being irradiated to 0.3 MGy and still retains 40% elongation even after being irradiated to 0.9 MGy, which is much better the control. It is expected that the formulated flame-retardant and radiation resistant EPDM materials could meet the requirements for use in radiation environments.

18/00258 Numerical investigation on the self-ignition behaviour of coal dust accumulations: the roles of oxygen, diluent gas and dust volume
Wu, D. *et al*. *Fuel*, 2017, 188, 500–510.
Self-ignition of coal dust deposits poses a higher risk of fires in oxygen-enriched oxy-fuel combustion systems. This work developed a numerical method, using the commercial software COMSOL Multiphysics, to investigate self-ignition behaviour of coal dust accumulations with a main emphasis on the roles of oxygen, diluent gas and dust volume. A one-step second-order reaction kinetic model considering both coal density and oxygen density is used to estimate reaction rate using the kinetic parameters from previously conducted hot-oven tests. This model is validated to predict the transient temperature and concentration profiles of South African coal dusts until ignition. The computed self-ignition temperatures of dust volumes show a good agreement with experimental results. In addition, it is found that the inhibiting effect of carbon dioxide is comparatively small and oxygen consumption increases dramatically after ignition. Parameter analysis shows that the heating value and kinetic parameters have a comparatively pronounced effect on self-ignition temperature. The model provides a satisfactory explanation for the dependence of self-ignition behaviour on gas atmospheres, thus helping to further understand the fire risk of self-ignition in oxy-fuel combustion systems.

18/00259 The role of CFD combustion modelling in hydrogen safety management – VI: validation for slow deflagration in homogeneous hydrogen-air-steam experiments
Rakhimov, A. C. *et al*. *Nuclear Engineering and Design*, 2017, 311, 142–155.
Large quantities of hydrogen can be generated during a severe accident in a water-cooled nuclear reactor. When released in the containment, the hydrogen can create a potential deflagration risk. The dynamic pressure loads resulting from hydrogen combustion can be detrimental to the structural integrity of the reactor. Therefore, accurate prediction of these pressure loads is an important safety issue. In previous papers, the authors validated a computational fluid dynamics (CFD) based method to determine the pressure loads from a fast deflagration. The combustion model applied in the CFD method is based on the turbulent flame speed closure (TFC). In their last paper, the authors presented the extension of this combustion model, extended turbulent flame speed closure (ETFC), and its validation against hydrogen deflagration experiments in the slow deflagration regime. During a severe accident, cooling water will enter the containment as steam. Therefore, the effect of steam on hydrogen deflagration is important to capture in a CFD model. The primary objectives of the present paper are to further validate the TFC and ETFC combustion models, and investigate their capability to predict the effect of steam. The peak pressures, the trends of the flame velocity, and the pressure rise with an increase in the initial steam dilution are captured reasonably well by both combustion models. In addition, the ETFC model appeared to be more robust to mesh resolution changes. The mean pressure rise is evaluated with 18% under-prediction and the peak pressure is evaluated with 5% accuracy, when steam is involved.

09 PROCESS HEATING, POWER AND INCINERATION

Energy applications in industry

18/00260 A new model for reliability optimization of series-parallel systems with non-homogeneous components
Feizabadi, M. and Jahromi, A. E. *Reliability Engineering & System Safety*, 2017, 157, 101–112.
In discussions related to reliability optimization using redundancy allocation, one of the structures that has attracted the attention of many researchers, is series-parallel structure. In models previously presented for reliability optimization of series-parallel systems, there is a restricting assumption based on which all components of a subsystem must be homogeneous. This constraint limits system designers in selecting components and prevents achieving higher levels of reliability. In this paper, a new model is proposed for reliability optimization of series-parallel systems, which makes possible the use of non-homogeneous components in each subsystem. As a result of this flexibility, the process of supplying system components will be easier. To solve the proposed model, since the redundancy allocation problem (RAP) belongs to the NP-hard class of optimization problems, a genetic algorithm (GA) is developed. The computational results of the designed GA are indicative of high performance of the proposed model in increasing system reliability and decreasing costs.

18/00261 An energy management approach for the mechanical manufacturing industry through developing a multi-objective energy benchmark
Cai, W. *et al*. *Energy Conversion and Management*, 2017, 132, 361–371.
Energy benchmark has been recognized as an effective analysis methodology and management tool of the energy usage. With wide distribution and large energy consumption in low efficiency, mechanical manufacturing industry possesses considerable energy-saving potential. However, there are few effective methods available for developing an energy benchmark in the mechanical manufacturing industry due to complexity and variety of energy-consumption processes resulting in the waste of massive energy. To achieve energy management and energy-efficient improvement in the mechanical manufacturing industry, this paper proposes a novel method for developing a multi-objective energy benchmark based on the energy consumption forecast and integrated assessment. Energy consumption databases, as an important part of the energy benchmark, are established to provide long-term use after establishment. Meanwhile, an energy consumption model of the whole production processes is built laying the foundation of the energy acquirement. The multi-objective energy benchmark could be determined through integrated assessment method of TOPSIS synthetically considering the real production requirements. In addition, the case study shows the practicability of the energy benchmark method for energy management and a potential energy saving of 21.3%.

18/00262 Can an emission trading scheme promote the withdrawal of outdated capacity in energy-intensive sectors? A case study on China's iron and steel industry
Zhu, L. *et al*. *Energy Economics*, 2017, 63, 332–347.
Outdated capacity and substantial potential for energy conservation are the two main features of energy-intensive sectors in developing countries. Such countries also seek to implement market-based options to further control domestic carbon emissions as well as to promote the withdrawal of outdated capacity and upgrade production level. This paper presents a quantitative assessment of the emission trading scheme for China's iron and steel industry. The diverse array of normal and outdated capacities was modelled in a two-country, three-good partial equilibrium model. Simulation results show that the abatement potential can be underestimated if the energy-saving effects that result from emission abatement are not considered. In the scenario analysis, it was demonstrated that the free allocation of allowances can cause a competitiveness distortion among domestic normal and outdated capacities. Given the government's intention to promote outdated capacity withdrawal and production-level upgrading, an output-based allocation approach is strongly suggested for China's iron and steel sector.

18/00263 Comparison of the catalytic effects of eight industrial wastes rich in Na, Fe, Ca and Al on anthracite coal combustion

Cheng, J. *et al. Fuel*, 2017, 187, 398–402.

The catalytic effects of eight industrial wastes rich in Na, Fe, Ca and Al on Jincheng anthracite coal combustion were compared. The thermogravimetric experiments showed that Na-rich brine sludge (BS) and salt sludge (SS) exhibited better catalytic effects on coal combustion than Fe-rich iron mud (IM) and steel residue (SR). However, IM and SR exhibited better catalytic effects than Ca-rich white lime mud (WLM) and calcium carbide residue (CCR). Among the eight industrial wastes, Al-rich alumina residue (AR) and aluminium slag (AS) demonstrated the worst catalytic effects. BS, which contains more Na (mainly in the form of NaCl, which was equivalent to Na_2O with a content of 13.14%) than SS (mainly in the form of NaCl and $Na_3Mg(CO_3)_2Cl$, which were equivalent to Na_2O with a content of 7.64%) does, reduced the ignition temperature of Jincheng coal from 582 to 561 °C because of the promoted transfer of oxygen to the carbon surface through the cyclic oxidation and reduction reactions between Na_2O and Na_2O_2. IM, which contains more Fe (mainly in the form of γ-Fe_2O_3, which was equivalent to Fe_2O_3 with a content of 92.22%) than SR (mainly in the form of Fe_2SiO_4 and α-Fe, which were equivalent to Fe_2O_3 with a content of 8.29%) does, reduced the ignition temperature of Jincheng coal to 569 °C as a consequence of the enhanced transfer of oxygen to the carbon surface through the cyclic oxidation and reduction reactions between FeO and Fe_2O_3.

18/00264 Energy efficiency barriers in commercial and industrial firms in Ukraine: an empirical analysis

Hochman, G. and Timilsina, G. R. *Energy Economics*, 2017, 63, 22–30.

Improvement in energy efficiency is one of the main options to reduce energy demand and greenhouse gas emissions. However, large-scale deployment of energy-efficient technologies is constrained by several factors. Employing a survey of 509 industrial and commercial firms throughout Ukraine and a generalized ordered logit model, the authors quantified the economic, behavioural, and institutional barriers that may impede the deployment of energy-efficient technologies. This analysis shows that behavioural barriers resulted from lack of information, knowledge, and awareness are major impediments to the adoption of energy-efficient technologies in Ukraine, and that financial barriers may further impede investments in these technologies especially for small firms. This suggests that carefully targeted information provisions and energy audits will enhance Ukrainian firms' investments in energy-efficient technologies to save energy consumption, improve productivity, and reduce carbon emissions from the productive sectors.

18/00265 Energy optimization and analysis modeling based on extreme learning machine integrated index decomposition analysis: application to complex chemical processes

Geng, Z. *et al. Energy*, 2017, 120, 67–78.

Energy optimization and analysis of complex chemical processes play a significant role in the sustainable development procedure. In order to deal with the high-dimensional and noise data in complex chemical processes, this paper presents an energy optimization and analysis method based on extreme learning machine integrating the index decomposition analysis. First, index decomposition analysis has been used to decompose the high-dimensional data to three energy performance indexes of the activity effect, the structure effect and the intensity. And then, those indexes and the production/conductivity of the chemical process are defined as inputs and outputs of the extreme learning machine respectively to build energy optimization and analysis model. Finally, the proposed method has been applied to optimizing and analysing energy status of the ethylene system and the purified terephthalic acid solvent system in complex chemical processes. The experiment results show that the proposed method has the characteristics of fast learning, stable network outputs and high model accuracy in handling with the high-dimensional data. Moreover, it can optimize energy of chemical processes and guide the production operation. In this experiment, the production of ethylene plants can be increased by 5.33%, and the conductivity of purified terephthalic acid plants can be reduced by 0.046%.

18/00266 Improving photofermentative biohydrogen production by using intermittent ultrasonication and combined industrial effluents from palm oil, pulp and paper mills

Budiman, P. M. *et al. Energy Conversion and Management*, 2017, 132, 110–118.

An ultrasonication technique was applied intermittently on photofermentation broth during the first 6 h of photofermentation to improve biohydrogen production by using *Rhodobacter sphaeroides* NCIMB8253. In this research, photofermentation broth consisted of a combination of palm oil (25%, v/v), pulp and paper (75%, v/v) mill effluents as well as liquid inoculum. The effects of amplitude (10, 20 and 30%, A) and ultrasonication duration (5, 10 and 15 min, T) were investigated in terms of their influences on photofermentative biohydrogen yield and total chemical oxygen demand (COD_{total}) removal. The recommended ultrasonication parameters were found at the middle range of amplitude and duration (A20T10). Using A20T10 intermittent treatment, the production of biohydrogen could be maximized up to 14.438 mL H_2/mL_{medium} with a COD_{total} removal and light efficiency of 52.2% and 7.412%, respectively. By comparing the treatment without intermittent ultrasonication, an increase of biohydrogen yield by 44.6% was achieved in A20T10 treatment. A total energy input of 306.1 J/mL (A20T10 treatment) was supplied to improve substrate consumption and light distribution during the photofermentation, which led to the increase of biohydrogen yield.

18/00267 Influence of surfactant and electrolyte concentrations on surfactant adsorption and foaming characteristics

Yekeen, N. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 612–622.

Surfactant adsorption and foaming characteristics are influenced by surfactant concentration and presence of inorganic electrolytes. Hence, it should be possible to optimize the performance of the surfactants in subsurface applications by understanding the influence of these parameters on surfactants. This study investigates the adsorption of sodium dodecyl sulfate (SDS) on kaolinite as a function of surfactant concentration and added electrolyte (NaCl, $CaCl_2$ and $AlCl_3$) concentration. Influence of temperature on the electrolyte and surfactant interactions was also examined. Adsorption isotherms were obtained using surfactant concentrations higher and lower than the critical micelle concentration (CMC). Surfactants adsorption on kaolinite was determined using a surface tension technique and two phase titration methods. Adsorption data were analysed by fitting with Langmuir and Freundlich adsorption isotherms. The foam was generated by dispersing CO_2 gas into the surfactant solution through a porous stone. Foam half-life and the rate of foam collapse as function of time was monitored. The adsorption of SDS by kaolinite increases with the increasing concentration of NaCl and $CaCl_2$ and decreasing temperature. However, adsorption in presence of $AlCl_3$ shows different behaviour. The adsorption remains constant irrespective of the increasing $AlCl_3$ concentration. Results show that the adsorption of SDS onto kaolinite in presence and absence of salts follows the Langmuir isotherm models. Salts containing trivalent ions and divalent ions ($AlCl_3$ and $CaCl_2$) were found to increase SDS adsorption on kaolinite and decrease bubbles stability compared to salts containing mono ions (NaCl). The order of increase in surfactant adsorption and bubble coalescence in presence of salts is as follows: $AlCl_3 > CaCl_2 >$ NaCl. There was an optimum surfactant concentration corresponding to maximum foam stability beyond which there was either a reduction or no significant changes in foam stability. This concentration decreases in presence of salts, except for $AlCl_3$ and high concentrations of NaCl (5 wt%) and $CaCl_2$ (1 wt%). The presence of salt improved foam generation and bubble stability at SDS concentration below the CMC. Above CMC, the bubble coalescence inhibition and foam stability decreased in the presence of salt. Decrease in surfactant surface tension and CMC, the screening effect of electrostatic double layer (EDL) by salts and the ability of SDS to form a complex with divalent (Ca^{2+}) and trivalent (Al^{3+}) cations are critical factors affecting SDS adsorption and foaming behaviours in presence of $AlCl_3$, $CaCl_2$ and NaCl salts. The results of this study have wide applications in the design, implementation and optimization of chemical EOR in the field.

18/00268 Optimal scheduling of demand responsive industrial production with hybrid renewable energy systems

Wang, X. *et al. Renewable Energy*, 2017, 100, 53–64.

This paper presents a methodology for the application of real-time optimization techniques to the problem of optimally scheduling and managing the interaction between electricity providers and users so that the grid and loads can come to an agreement to achieve optimal economic performance. The energy flows in typical industrial processes (e.g. chlor-alkali production) are simulated to illustrate day-ahead scheduling and contract following behaviours, as well as real-time demand response management. A communication and incentive scheme is first proposed for the complete energy scheduling process. Energy management strategies are then developed to realize the objectives of meeting production requirements while minimizing the overall operating and environmental costs through producing, purchasing and selling electricity. The energy contract following and demand response policies are also integrated into the proposed methodology, which appear to reduce uncertainties and help maintain the reliability of the grid.

18/00269 Preparation of high-purity nano-$CaCO_3$ from steel slag

Jo, H. *et al. Energy*, 2017, 120, 884–894.

Indirect carbonation is a suitable method for carbon dioxide (CO_2) removal from the environment, and it requires an acid to dissolve the calcium ions and a base to precipitate the formed calcium carbonate ($CaCO_3$). A new method to produce high-purity nano-$CaCO_3$ ($nCaCO_3$) from steel slag using hydrochloric acid (HCl) and sodium hydroxide (NaOH) is reported here. The rate equation for the dissolution of calcium (Ca) in the slag was derived using a range of variables, such as temperatures, solid-to-liquid (S/L) ratio, and HCl concentration. The purified calcium hydroxide ($Ca(OH)_2$) was converted into $nCaCO_3$ (size: 80–120 nm, purity: 98.5%) by carbonation with CO_2, after impurities, such as iron (Fe), aluminium (Al), and Mg, were completely removed. An efficiency of 73% was obtained for the dissolution and precipitation steps when 0.50 M HCl and 1.0 M NaOH were employed to produce 1 ton/h of nano-$CaCO_3$ with a purity of 98.5 wt%. Recently, a sodium chloride (NaCl) electrolysis system with low energy requirement was proposed to simultaneously produce HCl and NaOH. Assuming 90% faradic efficiency in the aforementioned NaCl electrolysis, process energies of 916 and 1462 kWh/t$CaCO_3$ were obtained at potentials of 0.83 and 1.50 V, respectively.

18/00270 Theoretical neutron damage calculations in industrial robotic manipulators used for non-destructive imaging applications

Hashem, J. *et al. Progress in Nuclear Energy*, 2017, 94, 71–79.

This paper describes how to use MCNP to evaluate the rate of material damage in a robot incurred by exposure to a neutron flux. The example used in this work is that of a robotic manipulator installed in a high intensity, fast, and collimated neutron radiography beam port at the University of Texas at Austin's TRIGA Mark II research reactor. This effort includes taking robotic technologies and using them to automate non-destructive imaging tasks in nuclear facilities where the robotic manipulator acts as the motion control system for neutron imaging tasks. Simulated radiation tests are used to analyse the radiation damage to the robot. Once the neutron damage is calculated using MCNP, several possible shielding materials are analysed to determine the most effective way of minimizing the neutron damage. Neutron damage predictions provide users the means to simulate geometrical and material changes, thus saving time, money, and energy in determining the optimal setup for a robotic system installed in a radiation environment.

10 SPACE HEATING AND COOLING/HEAT PUMPS

18/00271 A complex roof incorporating phase change material for improving thermal comfort in a dedicated test cell

Guichard, S. *et al. Renewable Energy*, 2017, 101, 450–461.

The use of phase change materials (PCMs) as a building integrated thermal storage may contribute to improving building energy performances. This article focuses on the integration of PCMs in the roof with a non-ventilated air layer, in order to assess thermal performances of a dedicated test cell, especially for thermal comfort. An experimental equipment was set up at Reunion Island under tropical and humid climatic conditions. A mathematical model, based on the apparent heat capacity method is used to predict the actual impact of PCMs on energy consumption as well as thermal comfort. Once the comparisons are performed with simulations, the use of the psychrometric chart, predicted mean vote and predicted percentage of dissatisfied indexes, shows that in the tested configurations, thermal comfort can be improved. Indeed, as well as to enhance the thermal energy storage, the given configuration also reduce the solar radiation through the roof, due to the reflective properties of PCMs panel surfaces. A positive effect on inside air temperature of the full-scale experimental test cell is particularly observed.

18/00272 A comprehensive, multi-objective optimization of solar-powered absorption chiller systems for air-conditioning applications

Shirazi, A. *et al. Energy Conversion and Management*, 2017, 132, 281–306.

Solar heating and cooling (SHC) systems are currently under rapid development and deployment due to their potential to reduce the use of fossil fuel resources and to alleviate greenhouse gas emissions in the building sector – a sector which is responsible for ~40% of the world energy use. Absorption chiller technology (traditionally powered by natural gas in large buildings), can easily be retrofitted to run on solar energy. However, numerous non-intuitive design choices must be analysed to achieve the best techno-economic performance of these systems. To date, there has been little research into the optimal configurations among the long list of potential solar-driven absorption chiller systems. To address this lack of knowledge, this paper presents a systematic simulation-based, multi-objective optimization of three common, commercially available lithium bromide–water absorption chillers – single-effect, double-effect and triple-effect – powered by evacuated tube collectors (ETCs), evacuated flat plate collectors (EFPCs), and concentrating parabolic trough collectors (PTCs), respectively. To the best of authors' knowledge, this is the first study of its kind that compares the optimized designs of the most promising configurations of solar-assisted absorption chillers against a common set of energy, economic, and environmental metrics from a holistic perspective. A simulation model of these three configurations is developed using TRNSYS 17. A combined energy, economic, and environmental analysis of the modelled systems is conducted to calculate the primary energy use as well as the levelized total annual cost of each plant, which are considered as two conflicting objective functions. By coupling TRNSYS and MATLAB, a multi-objective optimization model is formulated using a genetic algorithm to simultaneously minimize these objectives, thereby determining a set of optimal Pareto solutions corresponding to each SHC configuration. The performance of the proposed systems at their optimal designs is then compared to that of a reference conventional system. A sensitivity analysis is also performed to assess the influence of fuel cost, capital cost of innovative components, and the annual interest rate on the Pareto front of optimal solutions. Overall, the optimization results reveal that of the proposed configurations, the SHC double-effect chiller has the best trade-off between the energetic, economic and environmental performance of the system, having a total cost of ~0.7–0.9 M$ per year and reducing the annual primary energy use and CO_2 emissions by 44.5–53.8% and 49.1–58.2% respectively (relative to the reference conventional system). With the high capital cost associated with these systems, government subsidies and incentives are still required in order for them to achieve satisfactory payback times and become cost-competitive with conventional HVAC systems.

18/00273 A new solution for thermal interference of vertical U-tube ground heat exchanger for cold area in China

Li, X.-Y. *et al. Geothermics*, 2017, 65, 72–80.

This paper presents a new solution to reduce the thermal interference of vertical U-tube ground heat exchanger (UGHE): pipe insulation installed on the upward branch pipe of the U-tube. Three-dimensional numerical models of the UGHE with and without pipe insulation were developed to simulate the heat transfer process around the UGHE. The models were verified with previously published data. The effects of pipe insulation on outlet temperature, soil temperature, heat exchange rate per unit length of borehole depth and soil temperature recovery ratio were investigated. The effects of inlet velocity of heat transfer fluid (HTF) and the thermal conductivity of backfill material were also studied to fully assess the effects of the insulation. The results indicate that the average outlet temperature of HTF, soil temperature near the upward branch pipe and soil temperature recovery ratio all increased and the thermal interference can be effectively weakened when pipe insulation was installed.

18/00274 A novel ammonia-water combined power and refrigeration cycle with two different cooling temperature levels

Barkhordarian, O. *et al. Energy*, 2017, 120, 816–826.

A new ammonia–water cogeneration system is proposed to produce power and refrigeration outputs simultaneously, which combines Kalina power cycle and ejector refrigeration cycle. This cycle has two evaporators that can produce refrigeration output in two different temperature levels and capacities, in which the first evaporator pressure may be selected independently. This capability of the proposed cycle increases the number of possible applications while the complexity of the system does not vary much. Adjustable power to cooling ratio is another feature of this novel cycle, by changing the reboiler reflux ratio different power to cooling ratios can be reached. The cycle performance was evaluated by exergy efficiency, net power and refrigeration outputs. The effect of key parameters such as turbine inlet pressure, heat source temperature, condenser temperature, evaporation temperature and basic working solution ammonia concentration on the cycle performance have been investigated. It is found that the cycle's thermal performance is acceptable with exergy efficiency of 38.97%, effective exergy efficiency of 42.75% and thermal efficiency of 19% for the base case study.

18/00275 A passive decay-heat removal system for an ABWR based on air cooling

Mochizuki, H. and Yano, T. *Nuclear Engineering and Design*, 2017, 311, 35–42.

This paper describes the capability of an air cooling system (ACS) operated under natural convection conditions to remove decay heat from the core of an advanced boiling water reactor (ABWR). The motivation of the present research is the Fukushima severe accident (SA). The plant suffered damages due to the tsunami and entered a state of station blackout (SBO) during which seawater cooling was not available. To prevent this kind of situation, the authors proposed a passive decay heat removal system (DHRS) in the previous study. The plant behaviour during the SBO was calculated using the system code NETFLOW++ assuming an ABWR with the ACS. However, decay heat removal under an air natural convection was difficult. In the present study, a countermeasure to increase heat removal rate is proposed and plant transients with the ACS are calculated under natural convection conditions. The key issue is decreasing pressure drop over the tube banks in order to increase air flow rate. The results of the calculations indicate that the decay heat can be removed by the air natural convection after safety relief valves are actuated many times during a day. Duct height and heat transfer tube arrangement of the AC are discussed in order to design a compact and efficient AC for the natural convection mode. As a result, a four-pass heat transfer tubes with two-row staggered arrangement is the candidate of the AC for the DHRS under the air natural convection conditions. The heat removal rate is re-evaluated as a function of air mass velocity at the inlet of heat transfer tube banks.

18/00276 A review of energy storage technologies with a focus on adsorption thermal energy storage processes for heating applications

Lefebvre, D. and Tezel, F. H. *Renewable and Sustainable Energy Reviews*, 2017, 67, 116–125.

With depleting reserves of traditional fuels, there is a worldwide demand for alternative energy solutions. One of the most promising developing technologies is energy storage, as it provides the benefit of capturing available energy for use at a later time. This paper gives an overview of the numerous forms of energy storage technologies under investigation and development, with a focus on thermal energy storage through adsorption. The current materials tested for adsorption energy storage capabilities are presented together with their corresponding performances. The materials with the best thermal energy storage performance presented in the literature include hybrid adsorbents, adsorbents with salt impregnations, and adsorbents with alkaline additions, which provide energy densities of 226–309 kW h/m^3. Furthermore, the demonstrative projects and systems that currently use this technology are presented. Although thermal energy storage using adsorption processes is not currently economically viable, with continued material development and system optimization, this technology has the potential to become competitive in the near future.

18/00277 A semi-dynamic heat transfer model of hollow block ventilated wall for thermal performance prediction

Yu, J. *et al. Energy and Buildings*, 2017, 134, 285–294.

The hollow block ventilated wall is a new kind of ventilated wall, the exhaust air of HVAC system is used as the supply air to flow through the cavity of this wall in this paper. The heat or cool storage in the wall is reduced by using the heat recovery technology; the temperature of internal surface is lowered in summer and increased in winter, and the human thermal comfort is enhanced. A semi-dynamic heat transfer model of the ventilated wall is presented for thermal performance prediction. The dynamic optimized resistance-capacitance model and the number of transfer units model are joined together to develop the semi-dynamic heat transfer model of this ventilated wall. The experimental study is carried out for validating the semi-dynamic heat transfer model. The maximum relative error is 4.3% for mean internal and external surface temperatures, and it is 2.6% for the outlet air temperature of the cavity. The heat transfer model established for hollow block ventilated wall is fairly reasonable and possesses high accuracy. This model can be used to predict the surface temperature of the hollow block ventilated wall and the heat flux removed by the airflow in the cavity for performance evaluation.

18/00278 A study on thermal calculation method for a plastic greenhouse with solar energy storage and heating

Zhou, N. *et al. Solar Energy*, 2017, 142, 39–48.

Plastic greenhouse has been widely used in agriculture and horticulture due to its prolonging period for crops growth. In this work, an approach that stores solar energy in the daytime and provides heat by earth-tube at night was proposed, and then applied to a plastic greenhouse to elevate the inside air temperature. A one-dimensional dynamic model was established to assist the design of the solar energy storage and heating system and to evaluate the system performance. Using the model developed in Matlab, the date–hour change patterns of characteristic temperatures in the plastic greenhouse were obtained, through calculating the heat gains of various surfaces and heat storage by hour from solar radiation and solving the unsteady-state heat conduction equation in the structure components of the greenhouse. The calculated results show good agreement with the measured data, indicating that the method is valid and can be applied to the design of solar energy storage and heating system as well as the thermal performance analysis of greenhouses.

18/00279 Active-passive combined and closed-loop control for the thermal management of high-power LED based on a dual synthetic jet actuator

Deng, X. *et al. Energy Conversion and Management*, 2017, 132, 207–212.

In order to better solve the thermal management of high-power LED and facilitate its miniaturization, an active-passive combined heat dissipation method based on a dual synthetic jet actuator (DSJA) is proposed. Comparative analyses on heat dissipation characteristics and installation-space reductions of nine thermal management schemes are carried out. The results indicate that the temperature rapidly decreases and stabilizes once the actuator is activated. The heat dissipation effect based on DSJA is better than that based on synthetic jet actuator (SJA). The combination method with the vertical layout of DSJA makes the stable temperature of the LED and the installation space decrease 16 °C and 72.3% with respect to the commercial heat sink. Furthermore, a closed-loop system based on the combination method is developed to realize the autonomous control of the LED temperature within a setting temperature range. It is concluded that the operation duty cycle (ODC) reduces with the increase of the upper limit temperature, and there is an optimal impingement distance where the ODC is lowest of 29.1%. The closed-loop control will be greatly useful for the adaptive thermal management of electronic devices.

18/00280 Adapted computational method of energy level and energy quality evolution for combined cooling, heating and power systems with energy storage units

Jiang, X. Z. *et al. Energy*, 2017, 120, 209–216.

Current energy quality evaluation indexes mainly focus on depicting energy quality in systems whose character temperature and pressure are higher than environment. However, when the temperature and the pressure are lower than environment, these indexes sometimes fail to properly assess the energy quality of the system. Meanwhile, quoting different references or benchmarks in the calculation of some thermodynamics quantities, one of which is energy quality, may also confuse energy system designers. These situations will thereby result in potentially incomplete or partial evaluation of energy quality in complicated energy systems like combined cooling, heating and power (CCHP) systems. In this research, an adapted computational method of energy level which describes energy quality from thermal and mechanical perspectives has been proposed. In this method, energy quality of all-temperature and all-pressure conditions can be quantified without quoting different benchmarks, which allows thorough energy quality analysis for complicated energy systems. Energy quality evolution of a CCHP system with energy storage units (ESUs) has been discussed in terms of the proposed energy levels. The thermal energy quality evolution depicted by thermal energy level indicates that high energy level from waste heat of power generation units will cause large energy quality loss in the absorption refrigerator (AR), since the generation temperature in the AR confines the energy level in the generator to a comparatively low value. In the CCHP power generation unit, thermoacoustic engines prevail over gas turbines in energy quality conservation. Furthermore, mechanical energy level analysis shows that the absorption refrigerator and the absorption cooling storage units have higher mechanical energy levels than other components in CCHP systems due to the high vacuum conditions. Finally, an energy level matching map is provided to suggest matching strategies between waste heat sources and energy storage techniques in CCHP systems.

18/00281 Comparative study of two weir type cascade solar stills with and without PCM storage using energy and exergy analysis

Sarhaddi, F. *et al. Energy Conversion and Management*, 2017, 133, 97–109.

In this paper, the comparative study of energy and exergy performance of two weir type cascade solar stills with and without phase change material (PCM) storage in sunny and semi-cloudy days is carried out. The governing equations of energy analysis include a set of non-linear equations which is obtained by writing energy balance for the various components of a solar still (i.e. glass cover, brackish water, absorber plate, phase change materials). A detailed exergy analysis is carried out and various irreversibility rates in the solar still system and its exergy efficiency are introduced. In order to solve the governing equations a computer simulation program is developed. The results of a numerical simulation of the present study are in good agreement with the experimental data of previous literatures. The numerical results of the present study show that the energy and exergy performance of solar still without PCM storage is better than the solar still with PCM storage in sunny days. On the other hand, the solar still with PCM storage is

preferred for semi-cloudy days due to its better energy and exergy performance. The maximum value of the energy and exergy efficiencies of the solar still without PCM for a typical sunny day are 76.69% and 6.53%, respectively. While, the maximum energy and exergy efficiencies of the solar still with PCM for a sample semi-cloudy day are 74.35% and 8.59%, respectively. Furthermore, it is observed that the highest irreversibility rate belongs to the absorber plate and its value for the solar still without PCM on typical sunny day and the solar still with PCM on semi-cloudy days is 83.1% and 78.8% of the whole of system irreversibility rates, respectively. Whereas, the irreversibility rate of glass cover and brackish water can be neglected.

18/00282 Design of high-performance water-in-glass evacuated tube solar water heaters by a high-throughput screening based on machine learning: a combined modeling and experimental study

Liu, Z. *et al. Solar Energy*, 2017, 142, 61–67.

How to design water-in-glass evacuated tube solar water heater (WGET-SWH) with high heat collection rates has long been a question. Here, the authors propose a high-throughput screening (HTS) method based on machine learning to design and screen 3.538125×10^8 possible combinations of extrinsic properties of WGET-SWH, to discover promising WGET-SWHs by comparing their predicted heat collection rates. Two new-designed WGET-SWHs were installed experimentally and showed higher heat collection rates (11.32 and 11.44 MJ/m^2, respectively) than all the 915 measured samples in the authors' previous database. This study shows that the HTS method can be used to modify the design of WGET-SWH with just few knowledge about the highly complicated correlations between the extrinsic properties and heat collection rates of solar water heaters.

18/00283 Developing a performance evaluation model of organic Rankine cycle for working fluids based on the group contribution method

Su, W. *et al. Energy Conversion and Management*, 2017, 132, 307–315.

An organic Rankine cycle (ORC) model is presented in this paper to easily, quickly and inexpensively evaluate the performance potentials of various working fluids. When given molecular structure of working fluid, the normal boiling temperature, critical properties, liquid density and ideal gas heat capacity can be obtained via the existing group contribution methods (GCMs). Other properties required in the ORC model are calculated out by the thermodynamic relationships with the estimated properties of GCMs. Based on the calculated properties, four basic processes of the ORC including compression, evaporation, expansion and condensation are modelled. Meanwhile, the cycle parameters of 21 potential working fluids for typical ORC operating conditions are obtained from the molecular structures by the developed model. Compared with the REFPROP, the model shows sufficient accuracy for engineering purposes. The relative errors of thermodynamic properties and cycle parameters are less than 10% for most of working fluids. It is concluded that the proposed model can estimate the ORC characteristics of any pure working fluid only based on its molecular structure. Thus, a large amount of working fluids formed by the combination of groups can be directly screened by this model, and the optimal working fluids can be identified for a quick assessment in engineering field.

18/00284 Effect of $MgCl_2 \cdot 6H_2O$ phase change material on thermal insulation performance of carbon aerogels

Kazemi, A. *et al. Journal of Energy Storage*, 2017, 9, 59–68.

The aim of this work is to improve the thermal insulation performance (the time needed for the sample's top surface to reach 140 °C) of carbon aerogels (CAs) using phase change materials (PCMs). CAs were prepared through the carbonization of organic aerogels, synthesized by the sol-gel polymerization of a novolac solution under a solvent-saturated atmosphere. Field emission scanning electron microscopy (FE-SEM), N_2 adsorption and time-temperature history behaviour (insulation performance) characterization methods were used to investigate the morphology, microstructural and thermal properties of fabricated CAs, respectively. The CA sample prepared from the initial sol containing 20 wt% of novolac resin was identified as the proper CA sample to be the matrix for $MgCl_2 \cdot 6H_2O$-filled samples. The CAs were impregnated by $MgCl_2 \cdot 6H_2O$ using the immersion process. The influence of PCM content on the heat transfer of PCM-filled CAs was also investigated. Results presented here revealed that the amounts of filled PCMs can play an important role in improving the thermal performance of samples, in a specific temperature range (specifically around the melting point of PCM). Moreover, it was found that the low thermal conductivity of CA, combined with the high heat capacity of PCM, increased the time required to reach the top surface temperature of sample (140 °C). Increasing PCM contents enhanced the heat absorption capacity of the samples. In addition, the higher PCM contents resulted in the longer time interval of latent heat absorption. Furthermore, inhomogeneous impregnation of PCM in the structure of carbon aerogels resulted in more efficient structures, as, in this way, PCM can be located in the right place to meet required heat for phase change.

18/00285 Effect of oxygen defects on thermal conductivity of thorium-cerium dioxide solid solutions

Muta, H. *et al. Journal of Nuclear Materials*, 2017, 483, 192–198.

Thermal conductivity of thorium–cerium dioxide solid solutions has been measured and analysed using the relaxation time approximation. Despite the presence of oxygen defects, the partially reduced $Th_{0.8}Ce_{0.2}O_{1.97}$ exhibited higher thermal conductivity than the stoichiometric one, $Th_{0.8}Ce_{0.2}O_{2.00}$, showing the same tendency as that previously reported for $Th_{0.7}Pu_{0.3}O_{2-\delta}$. The increase in thermal conductivity with the oxygen defects can be explained by assuming that cerium ions have an average ionic radius of the ionic radii of Ce^{3+} and Ce^{4+} in the description of phonon–impurity scattering. This result indicates that the small reduction of $(Th,Pu)O_{2-\delta}$ fuel increases the thermal conductivity, especially at high temperatures.

18/00286 Effective use of thermal energy at both hot and cold side of thermoelectric module for developing efficient thermoelectric water distillation system

Al-Madhhachi, H. and Min, G. *Energy Conversion and Management*, 2017, 133, 14–19.

An efficient thermoelectric distillation system has been designed and constructed for production of drinkable water. The unique design of this system is to use the heat from hot side of the thermoelectric module for water evaporation and the cold side for vapour condensation simultaneously. This novel design significantly reduces energy consumption and improves the system performance. The results of experiments show that the average water production is 28.5 mL/h with a specific energy consumption of 0.00114 kW h/mL in an evaporation chamber filled with $10 \times 10 \times 30\,mm^3$ of water. This is significantly lower than the energy consumption required by other existing thermoelectric distillation systems. The results also show that a maximum temperature difference between the hot and cold side of the thermoelectric module is 42.3 °C, which led to temperature increases of 26.4 and 8.4 °C in water and vapour, respectively.

18/00287 Effects of sodium chloride on the thermal behavior of oxalic acid dihydrate for thermal energy storage

Han, L. *et al. Applied Energy*, 2017, 185, 762–767.

Oxalic acid dihydrate (OAD), which is inexpensive and has a high initial phase transition enthalpy, is a very promising phase change material. However, severe material leakage can occur owing to the large amount of steam generated when OAD is heated to melt. This behaviour subsequently degrades the thermophysical properties of OAD over time, thereby hindering further application of OAD. In the present study, NaCl was introduced as an additive in OAD to reduce its melting point. Results showed that a NaCl additive content of 9 wt% was the optimal amount to reduce the phase change temperature of OAD and produce sharp endothermal and exothermal peaks without reducing the phase change enthalpy significantly. Furthermore, minimal changes in the thermophysical properties of this mixture were observed after being subjected to 100 thermal cycles. The current findings are expected to broaden the application scope of OAD for thermal energy storage.

18/00288 Energy evaluation of rammed earth walls using long term in-situ measurements

Soudani, L. *et al. Solar Energy*, 2017, 141, 70–80.

Available throughout the world and used in construction for thousands of years, earthen materials are known to improve indoor air quality while keeping the internal temperature relatively stable. In Rhône-Alpes, France, the rammed earth technic is the most spread and consists in compacting layers of earth, one by one, within a framework. Current thermal standards, which are mainly based on thermal resistance of the material, urge to insulate walls. However, due to its interaction with its environment, and its couplings between heat and moisture transfers, the observed thermal behaviour of uninsulated rammed earth can be above the expectations. The objective of the paper is to highlight the living comfort provided by non-insulated rammed earth walls, for different orientations, from *in situ* measurements performed over more than 2 years. Winter, with low energy use for heating, and summer, with no cooling device, are studied. The study points out the important role of solar irradiance on the thermal balance of the house, and thus the importance of a good architecture.

18/00289 Energy performance and cost analysis of some borehole heat exchanger configurations with different heat-carrier fluids in mild climates

Emmi, G. *et al. Geothermics*, 2017, 65, 158–169.

The popularity of ground source heat pump systems for both heating and cooling has grown significantly over recent years. Ground heat exchangers are usually buried in the ground either vertically in

boreholes or horizontally in trenches. Antifreeze fluids in closed-loop systems are commonly used in these plants to protect them from freezing phenomena and also to reduce the total length of the ground exchangers. In fact, the use of antifreeze fluid allows the system to work below 0 °C which implies higher temperature difference between the heat-carrier fluid and the undisturbed ground, consequently the heat flux increases and the total length of the boreholes can be reduced. This study has been set out to investigate three types of layout system: two conventional heat pumps using pure water and water-glycol respectively as the secondary fluid and an innovative heat pump with a flooded evaporator using pure water. The results demonstrated that, for conventional heat pumps with dry evaporator, the use of anti-freeze additives in mild climates is convenient only in grid-shaped borehole fields with a heating-dominant thermal load. In all other cases, the use of pure water decreases the overall operating costs. In addition, flooded evaporator heat pumps using pure water as a secondary fluid on the ground loop proved to be the most cost-effective solution.

18/00290 Energy-storage properties of $Bi_{0.5}Na_{0.5}TiO_3$-$BaTiO_3$-$KNbO_3$ ceramics fabricated by wet-chemical method

Xu, Q. *et al*. *Journal of the European Ceramic Society*, 2017, 37, (1), 99–106.

$0.93Bi_{0.5}Na_{0.5}TiO_3$–$0.07BaTiO_3$ (BNTBT) and $KNbO_3$ (KN) powders with average particle size of ~50 and ~300 nm were synthesized by sol-gel method and hydrothermal method, respectively. Then, $(1-x)$(BNTBT)–xKN (BNTBT–KN, $x = 0$, 0.01, 0.03, 0.05, 0.07) ceramic samples were prepared using these two powder precursors. The structure, dielectric and energy-storage properties of BNTBT–KN ceramics were comprehensively investigated. All the ceramic samples were in single perovskite structure, indicating that KN can completely dissolve into BNTBT within the studied composition range. BNTBT–KN ceramics exhibited a high dielectric constant at room temperature, being in the order of 1430–1550. Ferroelectric hysteresis loops at room temperature became more slim with the increase of KN content, which largely improved energy-storage density and efficiency. For the composition of $x = 0.05$, the maximum recoverable energy-storage density reached 1.72 J/cm^3 under 16.8 kV/mm, which is superior to linear dielectrics and even some Pb-based systems. All these results demonstrate that 0.95BNTBT–0.05KN fabricated by wet-chemical method is a promising lead-free dielectric material for energy-storage capacitors.

18/00291 Experimental investigation and introduction of a similarity parameter for characterizing the heat and mass transfer in polymer desiccant wheels

Kang, H. and Lee, D.-Y. *Energy*, 2017, 120, 705–717.

The desiccant wheels made of a polymer desiccant were investigated at a low regeneration temperature with a purpose of utilizing low grade thermal energy. Three polymer desiccant wheels with different wheel thicknesses and different desiccant contents were tested for the dehumidification performance at various conditions of air velocity and rotation speed in a dedicated test facility placed in a climate chamber. The measured performance was compared with those of other desiccant wheels reported previously in literature. The polymer desiccant wheels were shown to display relatively higher dehumidification performance with smaller sensible temperature increase. In order to facilitate understanding the effects of the various test parameters, a single dimensionless parameter adapted from a theoretical work was introduced. It was shown that the effects of the wheel thickness, the air velocity and the rotation speed can be represented integratively by the single parameter. Similarities in the psychrometric states among the cases with different conditions were also addressed.

18/00292 Experimental investigation of quench and re-wetting temperatures of hot horizontal tubes well above the limiting temperature for solid–liquid contact

Takrouri, K. *et al*. *Nuclear Engineering and Design*, 2017, 311, 167–183.

Quench cooling of a hot dry surface involves the rapid decrease in surface temperature resulting from bringing the hot surface into sudden contact with a coolant at a lower temperature. Quench temperature is the onset of the rapid decrease in surface temperature and corresponds to the onset of destabilization of a vapour film that exists between the hot surface and the coolant. Situations involving quench cooling are encountered in a number of postulated accidents in Canada Deuterium Uranium CANDU reactors, such as the quench of a hot calandria tube in certain loss of coolant accidents (LOCA). If the calandria tube temperature is not reduced by initiation of quench heat transfer, then this may lead to subsequent fuel channel failure and for this accident knowledge of quench heat transfer characteristics is of great importance. In this study, a Water Quench Facility WQF has been designed and built at the Thermal Processing Laboratory at McMaster University and a series of experimental tests were carried out to investigate the quench of hot horizontal tubes using a vertical rectangular water multi-jet system. The tubes were heated to a temperature between 380 and 780 °C then cooled to the jet temperature. The temperature variation with time in tube circumferential and axial directions was measured. The two-phase flow behaviour and the propagation of the re-wetting front around and along the tubes were simultaneously observed using a high-speed camera. The effects of initial surface temperature, water subcooling (in the range 15–80 °C) and jet velocity (in the range 0.15–1.60 m/s) on the quench process were investigated. The quench and the re-wetting temperature (the temperature at which the liquid establishes wet contact with the solid) were found to greatly depend on water subcooling. One of the main findings in this study is the existence of a critical water subcooling range within which any small change in water subcooling has a considerable effect on both the quench and the re-wetting temperatures. Empirical correlations have been developed and provided good fit of the experimental data and agreed well with correlations developed by other researchers for curved surfaces. The quench temperature was found to decrease by increasing surface curvature and solid thermal conductivity. However, the re-wetting temperature is a weak function of both variables. Effect of spatial location on the surface of the tube was also studied. The stagnation point showed higher quench and re-wetting temperatures compared to other locations on the tube surface.

18/00293 Experimental verification of state space model and thermal performance analysis for active solar walls

Yu, G. *et al*. *Solar Energy*, 2017, 142, 109–122.

Building-integrated solar thermal system is a new tendency in the building sector. An active solar wall is studied in this paper, which integrates flat plate solar thermal collector and building wall. The performance of an active solar wall is predicted by the state space model and measured by experimental testing respectively. The calculated results by state space model agree well with the measured data from experimental testing, which indicates that state space model is valid. Thermal analysis for a particular solar wall is conducted in clear and cloudy days either in summer or winter respectively by state space model under Shanghai meteorological conditions and compared with the separate wall. The results indicate that: (1) integration has a little effect on the useful heat gains by solar collector. In clear summer days, the useful heat gains are less than the separate solar collector by about 2–3%; In clear winter days, the useful heat gain is greater than the separate solar collector by about 5–8%; (2) integration has great effect on the heat flow through walls. In clear summer, heat flow into the room through solar wall is significantly reduced by 55–63% than the separate wall. It is favourable to reduce cooling load. In winter, heat loss through solar wall is heavily reduced by about 80–88% than the separate wall. It is favourable to reduce the space heating load in winter.

18/00294 Experimental work to determine the effect of load pressure on the gel pack permeability of strong and weak preformed particle gels

Elsharafi, M. O. and Bai, B. *Fuel*, 2017, 188, 332–342.

Preformed particle gels (PPGs) have been widely applied to reduce the permeability of super-high permeability streaks/fractures. PPGs have an ability to decrease water production and increase sweep efficiency in mature oilfields. Either the success or failure of a PPG treatment depends largely on whether or not PPGs can effectively reduce the permeability of the fluid channels to an anticipated level. This work sought to investigate the influence of several factors on PPG blocking efficiency. A filtration model was designed to determine the permeability of PPGs packed in channels/fractures. Two types of PPGs were used for these filtration experiments: Daqing (DQ) and Liqui-Block 40 K. Particle sizes fell between 30 and 120 meshes. Results indicate PPG permeability decreased as load pressure increased. Additionally, PPGs with a larger particle size exhibited higher PPG pack permeability than PPGs with a smaller particle size. The PPG permeability with a lower brine concentration was more than the PPG pack permeability with a higher brine concentration when the PPG pack was not compressed by a piston. However, PPG pack permeability was less when using a lower brine concentration whether the PPG pack was compressed because the PPGs with higher brine concentration loss more water than the PPGs with the lower brine concentrations. According to the results the optimum gel pack with a preferred permeability can be designed by the right selection of the gel strength and correct particle size at reservoir pressure.

18/00295 Free-standing SWNTs/VO_2/Mica hierarchical films for high-performance thermochromic devices

Chen, Y. *et al*. *Nano Energy*, 2017, 31, 144–151.

Vanadium dioxide (VO_2) with reversible metal-insulator transition (MIT) is a promising energy-saving material for next-generation smart windows and infrared devices. However, the specific applications are largely limited by the relatively high critical temperature as well as the non-transferable grown-substrate. Herein, it is reported that such limitations can be overcome by directly growing VO_2 on layered mica

sheets and integrating with high transparent single-walled carbon nanotube (SWNT) films. The SWNTs/VO_2/mica hierarchical films can be peeled-off to form a free-standing ultra-thin optical window and can further be transferred to other substrates with high flexibility and transparency. By heating the SWNTs/VO_2 layer with a bias current, the MIT process of VO_2 film can be facilely modulated, achieving the reversible and dynamical regulation of the infrared transmission. Furthermore, by adjusting the bias current, it is possible to change the starting local temperature and shift the initial situation close to the 'phase transition boundary', resulting in the decreased energy barrier to trigger the MIT behaviour. This fascinating strategy overcomes the high critical temperature limit of VO_2 and avoids the bottle-neck problem in practical applications of VO_2 material, which demonstrates wide applications of this kind of device in the future.

18/00296 Freeze drying vs microwave drying – methods for synthesis of sinteractive thoria powders

Annie, D. *et al. Journal of Nuclear Materials*, 2017, 484, 51–58.

Thoria powders were synthesized by oxalate precipitation from an aqueous solution of the nitrate. The filtered precipitates were freeze dried or microwave dried before being calcined at 1073 K. The thoria powders obtained were characterized for crystallite size, specific surface area, bulk density, particle size distribution and residual carbon. Microstructure of the product was studied using scanning electron microscopy and transmission electron microscopy. Sinterability of the synthesized powders was studied by measuring the density of the sintered compacts. Powders that can be consolidated and sintered to densities ~96% theoretical density at 1773 K were obtained.

18/00297 Microencapsulated phase change materials for enhancing the thermal performance of Portland cement concrete and geopolymer concrete for passive building applications

Cao, V. D. *et al. Energy Conversion and Management*, 2017, 133, 56–66.

Concretes with a high thermal energy storage capacity were fabricated by mixing microencapsulated phase change materials (MPCM) into Portland cement concrete (PCC) and geopolymer concrete (GPC). The effect of MPCM on thermal performance and compressive strength of PCC and GPC were investigated. It was found that the replacement of sand by MPCM resulted in lower thermal conductivity and higher thermal energy storage, while the specific heat capacity of concrete remained practically stable when the phase change material (PCM) was in the liquid or solid phase. Furthermore, the thermal conductivity of GPC as function of MPCM concentration was reduced at a higher rate than that of PCC. The power consumption needed to stabilize a simulated indoor temperature of 23 °C was reduced after the addition of MPCM. GPC exhibited better energy saving properties than PCC at the same conditions. A significant loss in compressive strength was observed due to the addition of MPCM to concrete. However, the compressive strength still satisfies the mechanical European regulation (EN 206-1, compressive strength class C20/25) for concrete applications. Finally, MPCM-concrete provided a good thermal stability after subjecting the samples to 100 thermal cycles at high heating/cooling rates.

18/00298 Modeling and techno-economic analysis of the integration of a FC-based micro-CHP system for residential application with a heat pump

Sorace, M. *et al. Energy*, 2017, 120, 262–275.

This work aims to analyse the techno-economic performance of an integrated system for a residential combined heat and power (CHP) application, based on the integration of a fuel cell (FC) micro-cogeneration device coupled with a heat pump (HP). The main components of the system are: the FC unit, the HP and the thermal storage – required to cover the thermal peaks, mainly due to the domestic hot water demand. The analysis will be focused on the most diffused FC technologies for residential applications: a low-temperature polymer electrolyte membrane fuel cell (PEMFC) and a high-temperature solid oxide fuel cell (SOFC). FC-based cogeneration systems usually produce an electric power surplus respect to the thermal production, because of their high electrical efficiency. Currently, however, the households heating load exceeds significantly the electricity requirements, thus making difficult the sizing of a FC system for a single family house without including large electrical and thermal storages or high grid/boiler integration. The combination of a FC and a HP has been found to be an optimal solution to manage this problematic while achieving a reduction in the primary energy consumption and avoiding energy overproduction. In the proposed scenario the heat is exploited by feeding both the domestic hot water and a low-temperature radiant floor heating system operating between 35 and 45 °C. An energy and economic analysis has been performed to understand and to evaluate the plant feasibility. Results have pointed out that the best economic choice, with the current energy tariff scenario, is related to a small size FC-based CHP system able to produce enough electrical power to feed the HP plus a low electrical consumption (<1 kW electrical size), which corresponds to the base electrical household consumption (the electrical power which is near-always requested by the house). The electrical load is in fact deeply changing during the day (with one-minute variable peaks) and with a higher electrical production from the FC, most of the electrical power would be sold to the grid without no energy advantages. The best PEMFC configuration was able to reach a total efficiency of 75%: if compared to the case with separated energy generation (electricity from the grid and heat from a boiler) the saving is estimated in 3 years of payback for the current scenario (2015). With the SOFC system, thanks to its higher total efficiency equal to 81%, the primary energy consumption was reduced (−30% respect to PEMFC) with a consequent reduction in the operating costs. However, from an economic point of view, the payback still results extended because of its not competitive investment cost.

18/00299 Nanoporous anodic alumina oxide layer and its sealing for the enhancement of radiative heat dissipation of aluminum alloy

Lee, J. *et al. Nano Energy*, 2017, 31, 504–513.

Various types of nanoporous anodic aluminium oxide layers and their sealings were studied to enhance the thermal emissivity and hence improve the heat dissipation of aluminium alloy for energy application. Dissipating heat fluxes from the anodized aluminium surfaces were measured using a modified steady-state method and investigated with respect to the various nanoporous morphologies obtained with different anodizing conditions and sealing methods. Results show that the anodized nanoporous oxide layers significantly enhance the thermal emissivity and heat dissipation of aluminium alloy, compared to bare aluminium alloy, and such enhancement is further improved with sealings. A thicker nanoporous oxide layer anodized in oxalic acid results in higher thermal emissivity and better heat dissipation than that in sulfuric acid, showing a darker colour which is attributed to the more irregular and disordered pore size and pattern of the nanoporous oxide layer. The nanoporous oxide layer with cold NiF_2 or black sealing shows further enhancement in thermal emissivity and heat dissipation, demonstrating the highest enhancement in emissivity up to 0.906 in case of the nanoporous oxide layer anodized in oxalic acid with black sealing, which is seven times greater than that of bare aluminium. The nanoporous oxide layer with black sealing also results in the significant improvement of the cooling efficiency of a heat exchanger system of aluminium alloy by 36.4%, suggesting great energy saving for real energy application.

18/00300 Optimization of geothermal energy aided absorption refrigeration system – GAARS: a novel ANN-based approach

Tugcu, A. and Arslan, O. *Geothermics*, 2017, 65, 210–221.

The aim of this study is to optimize the geothermal energy aided absorption refrigeration system using NH_3–H_2O as the working fluid. A total of 3660 different designs, with different solution fractions and working parameters, were analysed by means of energy-exergy and net present value (NPV) analysis. The obtained data was modelled by a novel two-stage artificial neural network (ANN) with 14,650 data points. Of this, 10,248 points were used for training, and the remaining used for testing. The best topology of ANN were performed by using the back-propagation learning algorithm with three different variants such as Levenberg–Marquardt (LM), Pola–Ribiere conjugate gradient (CGP) and scaled conjugate gradient (SCG). According to ANN results, the error rates were determined in an acceptable range change between 0.07% and 6% for the engineering applications. The R^2 values of best network structures were calculated in higher acceptable range change between 0.9958 and 1.000 for LM. The optimum designs were determined using the obtained weights and biases of the best ANN topology, yielding a coefficient of performance (COP) and exergy efficiency (ε) of 0.5722 and 0.6201, respectively. NPV values were respectively calculated as US$1.778 million, $6.328 million and $27.183 million for quince, apple and grape.

18/00301 Performance analysis of heat pump and infrared–heat pump drying of grated carrot using energy-exergy methodology

Aktaş, M. *et al. Energy Conversion and Management*, 2017, 132, 327–338.

In this study, a hybrid drying system that combines all of the advantages of different drying methods was developed. This study aims to compare experimental results of a heat pump dryer (HPD) and an infrared assisted heat pump dryer (IRAHPD), to determine the energy and exergy efficiency of dryers and to analyse the drying kinetic of grated carrot for observing the effectiveness of the dryers. Samples were dried at 45 and 50 °C set temperatures and 0.5 m/s air velocity. According to dry basis calculation, initial moisture content amount was 7.06 g water/g dry matter and amount of final moisture content of dry matter was obtained as 0.14 g water/g dry matter. Energy efficiency varied between 5.3% and 50%. Minimum and maximum coefficients of performance

for the whole system (COP_{ws}) were 2.11 and 2.96, respectively. Maximum exergy efficiency was obtained 66.8% while minimum exergy efficiency was 31.6%. It was concluded that during the time to reach a stable state of system, the exergy efficiency increased in response to exergy loss decreases. This study shows a successful and efficient combination of heat pump and infrared heater in food drying.

18/00302 Performance enhancement of organic Rankine cycle with two-stage evaporation using energy and exergy analyses

Wang, J. *et al. Geothermics*, 2017, 65, 126–134.

The organic Rankine cycle (ORC) is promising in converting the low-medium grade thermal energy into power, but the efficiency is relatively low, which is mainly due to the poor temperature matching in the evaporator. Based on the single-stage evaporation of the ORC, the two stage evaporation strategy is proposed to improve the evaporation process between the heat source and the working fluid, with the heat source segmented into sections. The two-stage organic Rankine cycle (TSORC) was evaluated by the energy and exergy analyses. This paper aims to illuminate the two-stage evaporation mechanisms and optimize the cycle parameters. The results show that the two-stage evaporation enhances the evaporating temperature of the high-stage, thereby improving the evaporating process but deteriorating the expansion, condensation and pressurization processes. Overall, The TSORC tends to improve the system performance, which is at the cost of increasing the total thermal conductance, volumetric flow ratio, and the investment. A higher intermediate geothermal water temperature (IGWT) cannot effectively utilize the high-level heat source. There exists an optimal IGWT to maximize the objective function within the range of this study.

18/00303 Pumped thermal energy storage and bottoming system part A: concept and model

Abarr, M. *et al. Energy*, 2017, 120, 320–331.

This work introduces a new concept for a utility scale combined energy storage and generation system. The proposed design utilizes a pumped thermal energy storage (PTES) system, which also utilizes waste heat leaving a natural gas peaker plant. This system creates a low cost utility-scale energy storage system by leveraging this dual functionality. This Part A of a two-part paper presents a review of previous work in PTES as well as the details of the proposed integrated bottoming and energy storage system. A time-domain system model was developed in Mathworks R2016a Simscape and Simulink software to analyse this system. Validation of both the fluid state model and the thermal energy storage model are provided. The experimental results showed the average error in cumulative fluid energy between simulation and measurement was ±0.3% per hour. Comparison to a finite element analysis model showed <1% error for bottoming mode heat transfer. Part B of this two-part paper gives a detailed characterization of the integrated bottoming with energy storage system.

18/00304 Review of current state of research on energy storage, toxicity, health hazards and commercialization of phase changing materials

Chandel, S. S. and Agarwal, T. *Renewable and Sustainable Energy Reviews*, 2017, 67, 581–596.

Phase change materials (PCM) are widely used for energy storage applications worldwide. The objective of the study is to review the current state of research on PCM materials, energy storage, environmental aspects and identifying potential research areas which needs focus to make this technology widely marketable and economically promising. The paper presents PCM research status, material properties, microencapsulation, shape stabilization techniques, commercial applications and environmental issues and also covers areas which have not been given much attention in previous studies like toxicity, health hazards, fire retardation techniques and current market scenario. The study shows that salt hydrates are safe if carefully handled and commercial grade paraffins being flammable, release toxic vapours thus are potential health hazard so need to be used carefully. Further research on fire retardation of PCM is found lacking in literature. Critical issues to ensure long term performance, are discussed which will help researchers to identify appropriate PCM for different commercial applications. New innovative PCM materials are identified although these are not used in real applications as yet. The commercial potential of PCM products is presented which shows that these materials have promising solutions for textiles, heat or cold storage during transits, pain relief packs, vaccine and blood storage where maintenance of a critical temperature is important. These materials could significantly cut down the air conditioning demands in future provided the current challenges are met. With increased awareness and stricter environmental regulations in future, PCM market potential is expected to rise.

18/00305 Study on containment pressure response with passive containment cooling system performance under design basis accident

Wang, Y. and Yang, Y. *Progress in Nuclear Energy*, 2017, 94, 22–35.

The passive containment cooling system which utilizes natural phenomena to remove the energy released from reactor will prevent steel containment from overpressure during the postulated accident and provide long-term cooling to decrease the pressure and temperature of containment. The peak pressure in containment under the design basis accidents is important to the design and evaluation on the passive containment cooling system. In this paper, a dedicated code PCCSAP-3D for the evaluation on the performance of the passive containment cooling system is used to analyse the thermal-hydraulic transients in the containment of the advanced pressurized water reactor AP1000. Some factors are compared to study their *e* on the peak pressure of containment under the typical loss-of-coolant and main steam-line break accident. The results show that the amount of released coolant, the free volume and shell thickness of containment are dominant for containment pressure during the postulated accident, in comparison with the initial conditions. And the containment pressure response is more sensitive to internal initial conditions than to ambient conditions. The peak pressure under the postulated accidents is mainly contributed from rapid coolant release and it is not sensitive to the containment cooling performed by the passive containment cooling system.

18/00306 Temperature dependence of electrical conductivity of a green porcelain mixture

Lerdprom, W. *et al. Journal of the European Ceramic Society*, 2017, 37, (1), 343–349.

AC conductivity of a green porcelain body was investigated using impedance spectroscopy over a temperature range of 100–950 °C. The results showed that during the heating, conductivity at 100–200 °C increased mainly arising from H^+ and OH^- ions generated from adsorbing physical water. The activation energy increased below the dehydroxylation of clay resulting from movement of monovalent ions. At the dehydroxylation of clay, a combination of H^+, OH^- and monovalent ions dominated the conductivity. The activation energy rose to 1.14 eV (600–950 °C) controlled by diffusion of Na^+, and K^+ ions. During the cooling, conductivity showed single activation energy with 0.86 eV resulting from denser microstructure and change in mineralogical constituents and the heat treated porcelain sample showed higher electrical conductivity at the same temperature. Understanding conduction behaviour of the green porcelain enabled more accurate control of furnace temperature in flash sintering, a process which relies on electrical conductivity at high temperatures.

18/00307 Theoretical analysis on a new direct expansion solar assisted ejector-compression heat pump cycle for water heater

Chen, J. and Yu, J. *Solar Energy*, 2017, 142, 299–307.

This paper proposes a new direct expansion solar assisted ejector-compression heat pump cycle for water heater which can efficiently utilize the solar energy and air energy. The new cycle has two operation modes to be chosen according to the solar radiation intensity. The energetic and exergetic performance of the new cycle is analysed based on the built simulation model. Under the given conditions, the new cycle outperforms the basic ejector enhanced cycle in the heating coefficient of performance (COP) and heating capacity aspects by up to an average of 13.78% and 20.41%, respectively. The simulation results indicate that the operation mode A is more suitable for the low/zero solar radiation condition, while it's preferable to choose the operation mode B for the high solar radiation condition. The increase of the solar radiation intensity significantly benefits the performance of the new cycle, but decreases the system exergy efficiency. The exergy analysis also reveals that although the exergy destruction percentage of the solar collector increases with increasing the solar radiation intensity, the total exergy destruction percentage of other components decreases. The increase of the solar collector area always contributes to the performance improvement of the new cycle, but it should be kept in a proper range to guarantee the excellent performance and normal operation of the system.

18/00308 Theoretical and experimental study of aluminum foils and paraffin wax mixtures as thermal energy storage material

Reyes, A. *et al. Renewable Energy*, 2017, 101, 225–235.

This study analyses the effect of increased thermal conductivity in energy storage, using paraffin wax with 8% w/w of aluminium foils, obtained from waste materials. Three configurations previously not published of the aluminium foil were tested: stripes, horizontal perforated disks and vertical perforated foils. The aluminium foils doubled the thermal conductivity, achieving values of 0.63 W/mK, without significant statistical influence of the metallic configuration inside this material. Solidification time depended on the configuration

of the aluminium foils, where differences of up to 38% were detected between horizontal perforated disks and stripes. The equations for the solidification process were numerically solved in Matlab using the finite volume method, finding good agreement for the simulated output air temperature when compared with experimental values (relative error <10%). Later, a thermal energy accumulator was designed and assessed, which consisted of 12 cans with paraffin wax, using the horizontal perforated disks configuration. The energy stored by the phase change material was removed with air velocities between 0.5 and 1.5 m/s, reaching efficiencies close to 90% for the maximum air velocity.

18/00309 Thermal conductivity measurement of the He-ion implanted layer of W using transient thermoreflectance technique

Qu, S. *et al. Journal of Nuclear Materials*, 2017, 484, 382–385.

Transient thermoreflectance method was applied on the thermal conductivity measurement of the surface damaged layer of He-implanted tungsten. Uniform damages tungsten surface layer was produced by multi-energy He-ion implantation with thickness of 450 nm. Result shows that the thermal conductivity is reduced by 90%. This technique was further applied on sample with holes on the surface, which was produced by the He-implanted at 2953 K. The thermal conductivity decreases to 3% from the bulk value.

18/00310 Thermo-hydraulic performance of Therminol liquid phase heat transfer fluid in a ribbed tube of solar heater

Xu, W. *et al. Renewable Energy*, 2017, 101, 919–929.

Experiments and simulations on flow and heat transfer behaviour of Therminol 55 liquid phase heat transfer fluid have been conducted in a ribbed tube with outer and inner diameters of 25.0 and 20.0 mm, pitch and rib height of 12.0 and 1.0 mm, respectively. Experimental results show that the increase in heat transfer rate of the ribbed tube has a mean value of 2.24 times in the turbulent flow and in a range of 3.3–5.2 times in the laminar flow over the smooth tube at the test range. The measured average friction factor of the ribbed tube is in a range of 2.2–2.6 times over the smooth tube. The numerical results show that the heat transfer rate of the windward face wall is 1.34 times in excess of the heat transfer rate of the leeward face wall of ribs, which enhances heat transfer compared with smooth tube. In addition, correlations of the Nusselt number and friction factor in terms of Reynolds number and Prandtl number are determined, based on the curve fitting of the experimental data.

18/00311 Thermoelectric Skutterudite/oxide nanocomposites: effective decoupling of electrical and thermal conductivity by functional interfaces

Moure, A. *et al. Nano Energy*, 2017, 31, 393–402.

Nanocomposites that combine percolated nano-$CoSb_3$ semiconductors with isolated nano-oxide clusters are shown as an effective approach to decouple electrical and thermal conductivity in thermoelectric applications through the formation of functional interfaces. This type of decoupling is very important to increase the figure of merit (zT) of thermoelectrics and it is one of the greatest challenges searched by the community. The authors carry out an innovative synthesis of Skutterudite/oxide nanocomposites in air by high energy milling and sintering by spark plasma sintering, where functional interfaces are developed *in situ*. A confocal Raman microscopy study evidences unequivocally the appearance of a space charge layer at the Skutterudite/oxide interfaces characterized by a crystal lattice softening and a surprising enhanced Raman signal. The functional interfaces act as highly effective phonon scattering and trapping centres that highly reduce the thermal conductivity, while a high electrical conductivity is achieved by selective doping the Skutterudite phase. This approach leads to figures of merit *ca.* 1 for Te-doped $CoSb_3$. This work opens up new possibilities for the facile, large scale synthesis of well performing thermoelectric materials for medium range temperatures applications.

18/00312 Thermophysical properties of low cost lithium nitrate salts produced in northern Chile for thermal energy storage

Fernández, Á. G. and Gomez-Vidal, J. C. *Renewable Energy*, 2017, 101, 120–125.

In recent years, lithium-containing salts have been studied for thermal energy storage (TES) applications because of their excellent thermophysical properties. In solar power plants, lithium is seen as a way to improve the properties of state-of-the art molten salts used today. Lithium nitrate is a good candidate for sensible heat storage, because of its ability to increase the salt mixture's working temperature range. In the present research, thermophysical properties characterization of lithium nitrate containing salts, produced in Chile, have been carried out. Corrosion evaluations at 390 and 565 °C for 1000 h were performed for low chromium steel T22 and stainless steels (AISI 430 and AISI 316), respectively. Chemical composition of the salts including identification of corrosion products and impurities was determined and an estimation of the Chilean production costs is reported. The study shows a loss of thermal properties after the corrosion tests. The heat capacity was reduced, possibly caused by the formation of oxides at high temperatures. The partial thermal decomposition of the salt was probably produced by the incorporation of corrosion products from the steel.

18/00313 Use of fundamental condensation heat transfer experiments for the development of a sub-grid liquid jet condensation model

Buschman, F. X. and Aumiller, D. L. *Nuclear Engineering and Design*, 2017, 312, 147–160.

Condensation on liquid jets is an important phenomenon for many different facets of nuclear power plant transients and analyses such as containment spray cooling. An experimental facility constructed at the Pennsylvania State University, the High Pressure Liquid Jet Condensation Heat Transfer facility (HPLJCHT), has been used to perform steady-state condensation heat transfer experiments in which the temperature of the liquid jet is measured at different axial locations allowing the condensation rate to be determined over the jet length. Test data have been obtained in a pure steam environment and with varying concentrations of non-condensable gas. This data extends the available jet condensation data from near atmospheric pressure up to a pressure of 1.7 MPa. An empirical correlation for the liquid side condensation heat transfer coefficient has been developed based on the data obtained in pure steam. The data obtained with non-condensable gas were used to develop a correlation for the renewal time as used in the condensation suppression model developed by Young and Bajorek. This paper describes a new sub-grid liquid jet condensation heat transfer model. In the current work, mass and energy balance equations are solved in a marching scheme in each sub-grid node along the path of the jet trajectory. Jet specific condensation heat transfer closure relations are used. The jet sub-grid method has been implemented as a boundary condition in an in-house version of the sub-channel analysis code COBRA-TF (COBRA-IE). COBRA-IE fluid nodes provide the required vapour and non-condensable gas conditions for the heat transfer solution. The sub-grid model solves the liquid side heat transfer and the condensation rates for each volume in the sub-grid solution. These terms are summed along all of the sub-grid cells that pass through each COBRA-IE control volume to provide mass and energy transfer rates for the COBRA-IE solution. Results using the new jet injection boundary condition show an improved ability to simulate jet condensation experimental data.

18/00314 Validation of ANSYS CFX for gas and liquid metal flows with conjugate heat transfer within the European project THINS

Papukchiev, A. and Buchholz, S. *Nuclear Engineering and Design*, 2017, 312, 338–350.

Within the FP7 European project, Thermal Hydraulics of Innovative Nuclear Systems (THINS), numerical tools for the simulation of the thermal-hydraulics of next generation reactor systems were developed, applied and validated for innovative coolants. The Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS) gGmbH participated in THINS with activities related to the development and validation of computational fluid dynamics (CFD) and coupled System Thermal Hydraulics (STH) – CFD codes. High quality measurements from the L-STAR and TALL-3D experiments were used to assess the numerical results. Two-equation eddy viscosity and scale resolving turbulence models were used in the validation process of ANSYS CFX for gas and liquid metal flows with conjugate heat transfer. This paper provides a brief overview on the main results achieved at GRS within the project.

18/00315 Wind loads on buildings with vaulted roofs and side walls – a review

Natalini, B. and Natalini, M. B. *Journal of Wind Engineering and Industrial Aerodynamics*, 2017, 161, 9–16.

In this paper, a review of wind loads on cladded buildings with vaulted roofs was presented and the available information compared to the CIRSOC 102 treatment, an Argentinean code of practice whose recommendations are based on studies published in 1914. In general, the code treatment is not in agreement with current experimental evidence, although existing information regarding this particular typology is both limited and small in absolute terms. Potential criteria and values with which to update the code were discussed. However, it should be recognized that it is also necessary to improve the knowledge of these factors in order to design safer and more cost-effective structures.

18/00316 Worldwide trends on encapsulation of phase change materials: a bibliometric analysis (1990–2015)

Yataganbaba, A. *et al. Applied Energy*, 2017, 185, 720–731.

This study is planned as the first step of an investigation into the nano-encapsulation of phase change materials. The study combines a traditional literature review with data mining procedures by using bibliometric approach to identify the evolution of the knowledge structure related to encapsulation of phase change materials. Papers published from 1990 to 2015 in all journals indexed by the Scopus database were considered. Bibliometric methods and knowledge visualization technologies were employed to investigate publication activities based on the following indicators: year of publication, document type, language, country, institution, author, journal, keyword, number of citations. As a result of bibliometric analysis; 34,626 papers were determined with the keyword 'phase change material' and 1034 papers with the keyword 'encapsulation'. The number of publications on encapsulation of phase change materials have increased significantly after 2000. China, the USA and India are the most productive countries, while Tsinghua University and South China University of Technology from China are the most important institutions related to encapsulation. *Applied Energy* (39) is the most productive journal followed by *Energy Conversation and Management* (31). This is the first bibliometric analysis study on encapsulation of phase change materials. The results of this research support the idea that this type of bibliometric analysis would be a fruitful area as a first step for further works, not only associated with phase change materials. Further investigations into research fields are strongly recommended.

11 ENGINES

Power generation and propulsion, electrical vehicles

18/00317 A generalized kinetic model with variable octane number for engine knock prediction

Wang, Z. *et al. Fuel*, 2017, 188, 489–499.

A generalized research octane number (GRON) model, including 22 species and 21 reactions, has been developed to simulate the hydrocarbon oxidation with the goal of predicting engine knock. The simplicity of the model enables to represent gasoline with different octane numbers by adjusting the global low-temperature reaction rate. The model was validated against shock tube experimental data obtained over a wide range of conditions, including equivalence ratios from 0.5 to 2.0, initial pressures from 13 to 55 bar, and initial temperatures from 700 to 1250 K. Both gasoline engine knock and normal combustion were investigated using computational fluid dynamics (CFD) couple with the present GRON. The numerical results proved to be in good agreement with the experimental data. Both the cylinder pressure traces and the distribution of important radical species (CHO and OH) during knocking combustion can be predicted reasonably well. Compared to the CFD calculations using detailed mechanisms, the generalized kinetic model enables a reduction of the computational time by more than 90%.

18/00318 Advances and challenges in modeling high-speed turbulent combustion in propulsion systems

Gonzalez-Juez, E. D. *et al. Progress in Energy and Combustion Science*, 2017, 60, 26–67.

Combustion environments in propulsion systems involve the interaction of a variety of physics. In devices such as augmentors, ramjets and scramjets, such environments include the interaction between combustion, high-intensity turbulence, and/or strong flow compressions and expansions, physics which are termed here high-speed combustion. With this motivation in mind, this paper addresses: What are the problems encountered when modelling these interactions, or in other words, what are the problems of turbulent-combustion modelling? Do such interactions need modelling? What are the challenges when going from modelling low-speed- to high-speed-combustion problems? This work addresses these questions by summarizing several modelling studies of gaseous high-speed-combustion problems, and attempts to interpret some predictions in the context of the models' basic assumptions. Interestingly, the challenges to model high-speed combustion are such that a reader not interested in this topic but in the general one of modelling turbulent combustion may find the present paper useful.

18/00319 Calcium-magnesium-alumina-silicate (CMAS) resistance characteristics of $LnPO_4$ (Ln = Nd, Sm, Gd) thermal barrier oxides

Wang, F. *et al. Journal of the European Ceramic Society*, 2017, 37, (1), 289–296.

Calcium–magnesium–alumina–silicate (CMAS) attack has been considered as a significant failure mechanism for thermal barrier coatings (TBCs). As a promising series of TBC candidates, rare-earth phosphates have attracted increasing attention. This work evaluated the resistance characteristics of $LnPO_4$ (Ln = Nd, Sm, Gd) compounds to CMAS attack at 1250 °C. Due to the chemical reaction between molten CMAS and $LnPO_4$, a dense, crack-free reaction layer, mainly composed of $Ca_3Ln_7(PO_4)(SiO_4)_5O_2$ apatite, $CaAl_2Si_2O_8$ and $MgAl_2O_4$, was formed on the surface of compounds, which had positive effect on suppressing CMAS infiltration. The depth of CMAS penetration in $LnPO_4$ (Ln = Nd, Sm, Gd) decreased in the sequence of $NdPO_4$, $SmPO_4$ and $GdPO_4$. $GdPO_4$ had the best resistance characteristics to CMAS attack among the three compounds. The related mechanism was discussed based on the formation ability of apatite phase caused by the reaction between molten CMAS and $LnPO_4$.

18/00320 Comparison of in-cylinder combustion and heat-work conversion processes of vehicle engine under transient and steady-state conditions

Xu, Z. *et al. Energy Conversion and Management*, 2017, 132, 400–409.

To improve the actual performance of internal combustion engine (ICE), the transient behaviours of in-cylinder combustion and heat–work conversion processes of ICE were investigated and an optimization method was proposed. Based on an advanced turbocharged gasoline direct injection (TGDI) engine, the steady-state bench test, load-step test at constant-speed and vehicle road test were carried out. On this basis, the in-cylinder combustion and heat–work conversion processes of vehicle engine under load-step and vehicle driving conditions were compared with the steady-state results. By this means, the deviations of ICE transient performance from their steady-state values were demonstrated and also their impacts were revealed. The research results show that there is a satisfactory consistency of ICE performance especially the ignition advance angle under load-step and steady-state conditions. However, under vehicle driving conditions, the operating and control parameters gravely deviate from the steady-state values with large fluctuations, e.g. ignition advance angle is retarded largely under the sharp deceleration conditions. When the IMEP is below 4 bar, the ignition advance angle seriously deviates from the steady-state values, which results in large fluctuation of combustion characteristic parameters and finally leads to the decrease of heat-work conversion efficiency. Moreover, the fluctuation of excess air coefficient is one of the main reasons for the instability of ICE transient performance. To accurately control the ignition timing under low load and decrease the fluctuation of excess air coefficient is an effective way to improve the ICE performance under vehicle driving conditions.

18/00321 Deterioration of palm biodiesel fuel under common rail diesel engine operation

Chandran, D. *et al. Energy*, 2017, 120, 854–863.

Although numerous studies have shown the adverse effects of oxidized biodiesel and/or higher total acid number (TAN) and water content in biodiesel fuel on the degradation of fuel delivery materials, limited work has been reported to date to ascertain the presence of these factors under actual engine operation. Therefore, the aim here is to determine if these factors exist under common rail diesel engine (CRDE) operation. For this, an engine test-bed comprising a Toyota 1KD-FTV engine coupled to an eddy current dynamometer was operated under two different speed-load test cycles using palm biodiesel with 10.5 h of oxidation stability according to the Rancimat test. The results indicated that the biodiesel fuel samples were not oxidized while both TAN value and water content were unaffected at the end of the CRDE operations under both the test cycles. As such, emphasis should not only be placed solely on the acceleration of fuel delivery materials degradation due to biodiesel oxidation and/or greater TAN value and water content under engine operation. This study also demonstrated that biodiesel conductivity value is a more appropriate indicator of fuel deterioration level under CRDE operation which ultimately determines the compatibility between biodiesel and fuel delivery materials.

18/00322 Dynamic model linearization of two shafts gas turbine via their input/output data around the equilibrium points

Hadroug, N. *et al. Energy*, 2017, 120, 488–497.

The present paper deals with a linearization strategy of the non-linear model presenting a gas turbine with two shafts. Indeed, being able to describe and to explain the various phenomena involved and interacted in the dynamics of the turbines has a great impact in practice. Whereas; the modelling of the gas turbine using real data allows to approximate the variables of this non-linear system based on a linearization

approach. It is obvious that the advantage of this approach is to ensure the prediction and the monitoring of the gas turbine behaviour to assess its optimized control. In this paper the obtained results based on real data of onsite measurements allow to understand and to analyse the phenomena interacting in the gas turbine system, and therefore the prediction of its dynamic behaviour can be ensured.

18/00323 Effects of fuel injection parameters on emission characteristics of diesel engines operating on various biodiesel: a review

Mohamed Shameer, P. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 1267–1281.

Many researches have been carried out towards the reduction in noxious emissions from diesel engines. This paper reviews the studies on the outcomes of operating parameters discrepancy on the engine emission issues carried out by various authors in different diesel engines fuelled with biodiesel from different feedstocks. The main goal of this paper is to enlighten the momentous of injection parameters like injection timing and injection pressure on the engine emission characteristics. This paper touches upon the advancement and retardation methods of fuel injection timing and injection pressure to inspect the engine emission indicators such as carbon monoxide, hydrocarbon, oxides of nitrogen, smoke, particulate matter and carbon dioxide contents. Comparative evaluation has been conversed accompanied by apropos causes for the deviation of emission characteristics.

18/00324 Engine performance and emissions characteristics of a diesel engine fueled with diesel-biodiesel-bioethanol emulsions

Tan, Y. H. *et al. Energy Conversion and Management*, 2017, 132, 54–64.

In this research work, the experimental investigation of the effect of diesel–biodiesel–bioethanol emulsion fuels on combustion, performance and emission of a direct injection (DI) diesel engine are reported. Four kind of emulsion fuels were employed: B (diesel-80%, biodiesel-20% by volume), C (diesel-80%, biodiesel-15%, bioethanol-5%), D (diesel-80%, biodiesel-10%, bioethanol-10%) and E (diesel-80%, biodiesel-5%, bioethanol-15%) to compare its performance with the conventional diesel, A. These emulsion fuels were prepared by mechanical homogenizer machine with the help of Tween 80 (1% v/v) and Span 80 (0.5% v/v) as surfactants. The emulsion characteristics were determined by optical electron microscope, emulsification stability test, FTIR, and the physiochemical properties of the emulsion fuels which were all done by following ASTM test methods. The prepared emulsion fuels were then tested in diesel engine test bed to obtain engine performance and exhaust emissions. All the engine experiments were conducted with engine speeds varying from 1600 to 2400 rpm. The results showed the heating value and density of the emulsion fuels decrease as the bioethanol content in the blend increases. The total heating value of the diesel–biodiesel–bioethanol fuels were averagely 21% higher than the total heating value of the pure biodiesel and slightly lower (2%) than diesel fuel. The engine power, torque and exhaust gas temperature were reduced when using emulsion fuels. The brake specific fuel consumption for the emulsion fuels were observed to be higher in comparison to diesel, A. The CO_2 (carbon dioxide) and CO (carbon monoxide) emissions were reported to be lower than diesel oil. The effect of using emulsion fuels decreased the NO_x (nitrogen oxides) emissions at medium engine speeds, i.e. approximately 30.0%. Lesser NO_x emission was attributed by the reduction of cetane number of the diesel–biodiesel–bioethanol emulsion fuels' cetane number as the amount of bioethanol increases. However, the emissions of NO_x were found to increase gradually at low speed (~1600 rpm), high load; high speed (~2400 rpm), medium load conditions. It was found that the combustion performance and emissions of the diesel engine very much depend on the fuel, its emulsion combination types and engine operating conditions.

18/00325 Experimental and vehicle (on road) test investigations of spark-ignited engine performance and emissions using high concentration of MTBE as oxygenated additive

Schifter, I. *et al. Fuel*, 2017, 187, 276–284.

This study considers the effect of increasing methyl-tert butyl ether in regular gasoline (15, 25 and 51% volume) on the performance and combustion characteristics of spark ignited engines. A single cylinder engine, spark ignited was used. The engine in fully instrumented in order to measure all the relevant parameters, i.e. temperatures, pressures, exhaust emissions, intake air and fuel flows and indicating parameters like mass burned fuel. Results were compared with those obtained with a fleet of five model year 2003–2010 passenger cars. For that purpose FTP-74 tests were performed for the fuel containing 25% MTBE and compared with those obtained with the regular commercial gasoline. The gasoline-MTBE at 25% blend presents the lowest dispersion among the tested fuels, and the evolution of the instantaneous pressure with respect to the crank angle for each fuel, pointed out that no misfires occurred. The fuel with high contents MTBE (Blends 2 and 3) burn slightly later than the fuels formulated with typical MTBE contents around 11% volume. On the average, fuel economy seems to decrease as MTBE increases in accordance with the results observed using the single cylinder engine. The results shows no immediately adverse effects when the MTBE contents increases up to 51%, and a small reductions in NOx as the MTBE contents increases. The octane requirement of the tested vehicles may be controlled by the knock sensors that adjust the engine operating. Clearly the use of high contents of ethers (i.e. between 25% and 30% MTBE in volume) as a fuel constituent represents an alternative for fuel decarbonization in Mexico and can be an alternative way to reduce the use of fossil fuels.

18/00326 Experimental assessment of the fuel heating and the validity of the assumption of adiabatic flow through the internal orifices of a diesel injector

Salvador, F. J. *et al. Fuel*, 2017, 188, 442–451.

In this paper an experimental investigation on the heating experienced by the fuel when it expands through the calibrated orifices of a diesel injector is carried out. Five different geometries corresponding to the control orifices of two different commercial common-rail solenoid injectors were tested. An experimental facility was used to impose a continuous flow through the orifices by controlling the pressures both upstream and downstream of the restriction. Fuel temperature was controlled prior to the orifice inlet and measured after the outlet at a location where the flow is already slowed down. Results were compared to the theoretical temperature increase under the assumption of adiabatic flow (i.e. isenthalpic process). The comparison points out that this assumption allows to predict the fuel temperature change in a reasonable way for four of the five geometries as long as the pressure difference across the orifice is high enough. The deviations for low imposed pressure differences and the remaining orifice are explained due to the low Reynolds numbers (i.e. flow velocities) induced in these cases, which significantly increase the residence time of a fuel particle in the duct, thus enabling heat transfer with the surrounding atmosphere. A dimensionless parameter to quantify the proneness of the flow through an orifice to exchange heat with the surroundings has been theoretically derived and calculated for the different geometries tested, allowing to establish a boundary that defines beforehand the conditions from which heat losses to the ambient can be neglected when dealing with the internal flow along a diesel injector.

18/00327 Gas-particle flows and erosion characteristic of large capacity dry top gas pressure recovery turbine

Cai, L. *et al. Energy*, 2017, 120, 498–506.

Based on the erosion rate model and the particle rebound model of blade material obtained through accelerated erosion test under high temperature, systematic numerical simulations of the complex gas-particle flows in inlet volute and cascade of a large capacity gas pressure recovery turbine are performed in this paper. The influence of inlet volute structure and cascade channel structure on the aerodynamic performance and erosion characteristics of turbine is first investigated. Results show that although mixing flows and vortex flows are formed in turbine intake volute, total pressure loss of volute is less than 0.7% because of low gas velocity. Erosion damage on the trailing edge of nozzles and rotating blades is mainly caused by high-speed cutting behaviour of ash particles. The typical inlet volute structure results in an uneven erosion of first stage nozzles along circumferential direction. Nozzles located below the horizontal split are mainly eroded in blade root area, while erosion distribution of nozzles located above the horizontal split is irregular, and worse than the erosion degree of the lower half circle. Flow acceleration characteristics and cascade circumferential structure must be comprehensively considered so as to simultaneously improve the aerodynamic and anti-erosion performance of turbine.

18/00328 Ignition and combustion characteristics of *n*-pentanol–diesel blends in a constant volume chamber

Ma, Y. *et al. Applied Energy*, 2017, 185, 519–530.

Pentanol is considered as one of the most promising alternative biofuels due to its excellent physicochemical properties. The objective of this work was to compare the ignition and combustion characteristics of different *n*-pentanol/diesel blends in an optical constant volume combustion chamber. The tested fuels included 20% (D80P20) and 40% (D60P40) of *n*-pentanol blended with diesel in volume, and pure diesel (D100). Broadband chemiluminescence technique was used to measure the timing and location of spray ignition. A high-speed CCD camera with two ND8 dimmer lenses was used to capture the incandescence radiated from the soot particles during combustion. A wide range of experimental conditions was investigated. The ambient temperature ranged from 800 to 1200 K and the oxygen concentration ranging from 10% to 21%, covering both the conventional and low temperature combustion regimes. The results show that pure diesel has shorter ignition delay and distance comparing to pentanol blends. A larger blending proportion of pentanol D60P40 advances the ignition phase more than the D80P20 in low oxygen concentration conditions.

Due to the fuel-borne oxygen and the dilution effect, the natural flame luminosity is reduced significantly with the increase of pentanol ratio in most conditions except under the intermediate temperature region of 1000 K. In that condition, the shorter ignition delay and flame lift-off length of pentanol blends cause a slightly increase in the natural flame luminosity. The natural flame luminosity images showed that the oxygen-contained structure of pentanol could accelerate soot oxidation under all conditions. This indicates that pentanol blends could decrease final soot emissions in internal combustion engines.

18/00329 Impact of fuel molecular structure on auto-ignition behavior – design rules for future high performance gasolines

Boot, M. D. *et al. Progress in Energy and Combustion Science*, 2017, 60, 1–25.

At a first glance, ethanol, toluene and methyl tert-butyl ether look nothing alike with respect to their molecular structures. Nevertheless, all share a similarly high octane number. A comprehensive review of the inner workings of such octane boosters has been long overdue, particularly at a time when feedstocks for transport fuels other than crude oil, such as natural gas and biomass, are enjoying a rapidly growing market share. As high octane fuels sell at a considerable premium over gasoline, diesel and jet fuel, new entrants into the refining business should take note and gear their processes towards knock resistant compounds if they are to maximize their respective bottom lines. Starting from crude oil, the route towards this goal is well established. Starting from biomass or natural gas, however, it is less clear what dots on the horizon to aim for. The goal of this paper is to offer insight into the chemistry behind octane boosters and to subsequently distil from this knowledge, taking into account recent advances in engine technology, multiple generic design rules that guarantee good anti-knock performance. Careful analysis of the literature suggests that highly unsaturated (cyclic) compounds are the preferred octane boosters for modern spark-ignition engines. Additional side chains of any variety will dilute this strong performance. Multi-branched paraffins come in distant second place, owing to their negligible sensitivity. Depending on the type and location of functional oxygen groups, oxygenates can have a beneficial, neutral or detrimental impact on anti-knock quality.

18/00330 Impacts of additives on performance and emission characteristics of diesel engines during steady state operation

Khalife, E. *et al. Progress in Energy and Combustion Science*, 2017, 59, 32–78.

Depletion of fossil fuel resources and stringent emission mandates has spurred the search for improved diesel engines performance and cleaner combustion. One of the best approaches to solve these issues is to use biodiesel/diesel additives. The effects of biodiesel/diesel additives on the performance and emissions of diesel engines were comprehensively reviewed throughout this article. The additives reviewed herein were classified into five categories, i.e. oxygenated additives, metallic and non-metallic based additives, water, antioxidants, and polymeric-based additives. The effects of each category on the engine performance (i.e. brake specific fuel consumption and brake thermal efficiency) and emissions (i.e. CO, NO_x, HC and PM) were exclusively summarized and discussed. Furthermore, various strategies used for adding water like water–diesel emulsion, direct water injection, and adding water into the inlet manifold were illustrated and their pros and cons were completely scrutinized. Finally, opportunities and limitations of each additive considering both engine performance and combustion benignity were outlined to guide future research and development in the domain.

18/00331 In-cylinder pressure-based air-fuel ratio control for lean burn operation mode of SI engines

Kumar, M. and Shen, T. *Energy*, 2017, 120, 106–116.

In this paper, an in-cylinder air–fuel ratio control problem for lean burn mode operation of spark ignition engine is investigated with cycle-based model considering the cycle-to-cycle coupling effects of residual gas compositions. The statistical properties of parameter variation of the cyclic transient model are calibrated based on experiments of lean burn operating modes. With the calibrated model, a model-based predictive control strategy is proposed to improve the preciseness of in-cylinder air—fuel ratio at lean-burn operation including transient operation. To analyse the combustion parameters and its stability, the cycle-based indicators, such as heat transfer, indicated mean effective pressure (IMEP), combustion efficiency, residual gas fraction, peak pressure, crank angle at 50% heat release (CA50) and NO_x emission are adopted. The consecutive cycle co-relation is also addressed to analyse the stochastic behaviour at lean combustion. Finally, experimental validation are performed and demonstrated on a full-scaled gasoline engine test bench to show the effectiveness of proposed lean-mode control scheme and combustion stabilities.

18/00332 Modelling of blended diesel and biodiesel fuel droplet heating and evaporation

Al Qubeissi, M. *et al. Fuel*, 2017, 187, 349–355.

The paper presents a new approach to the modelling of heating and evaporation of dual-fuel droplets with a specific application to blends of biodiesel (represented by the widely used soybean methyl ester, SME) and diesel fuels in conditions representative of internal combustion engines. The original compositions, with up to 105 components of diesel and biodiesel fuels, are replaced with a smaller number of components and quasi-components using the recently introduced multi-dimensional quasi-discrete (MDQD) model. Transient diffusion of these components and quasi-components in the liquid phase and temperature gradient and recirculation inside droplets are taken into account. The results are compared with the predictions of the case when blended biodiesel/Diesel fuel droplets are represented by pure biodiesel fuel or pure Diesel fuel droplets. It is shown that droplet evaporation time and surface temperature predicted for 100% SME, representing pure biodiesel fuel, are close to those predicted for pure diesel fuel. Also, it is shown that the approximations of the actual compositions of B5 (5% SME and 95% diesel) and B50 (50% SME and 50% Diesel) dual-fuels by 17 quasi-components/components, using the MDQD model, lead to under-predictions in droplet lifetimes by up to 9% and 4%, respectively, under the same engine conditions. The application of the latter model has resulted in above 83% reduction in CPU time compared to the case when all 105 components are taken into account using the discrete component model.

18/00333 Performance and emissions of gasoline blended with terpineol as an octane booster

Vallinayagam, R. *et al. Renewable Energy*, 2017, 101, 1087–1093.

This study investigates the effect of using terpineol as an octane booster for gasoline fuel. Unlike ethanol, terpineol is a high energy density biofuel that is unlikely to result in increased volumetric fuel consumption when used in engines. In this study, terpineol is added to non-oxygenated FACE F gasoline (research octane number = 94.5) in volumetric proportions of 10%, 20% and 30% and tested in a single cylinder spark ignited engine. The performance of terpineol blended fuels are compared against a standard oxygenated EURO V (ethanol blended) gasoline. It was determined that the addition of terpineol to FACE F gasoline enhanced the octane number of the blend, resulting in improved brake thermal efficiency and total fuel consumption. For FACE F + 30% terpineol, break thermal efficiency was improved by 12.1% over FACE F gasoline at full load for maximum brake torque operating point, and similar performance as EURO V gasoline was achieved. Due to its high energy density, total fuel consumption was reduced by 6.2% and 9.7% with 30% terpineol in the blend when compared to FACE F gasoline at low and full load conditions, respectively. Gaseous emissions such as total hydrocarbon and carbon monoxide emission were reduced by 36.8% and 22.7% for FACE F + 30% terpineol compared to FACE F gasoline at full load condition. On the other hand, nitrogen oxide and soot emissions are increased for terpineol blended FACE F gasoline when compared to FACE F and EURO V gasoline.

18/00334 Quantitative analysis on the thermodynamics processes of gasoline engine and correction of the control equations for heat-work conversion efficiency

Yuan, Z. *et al. Energy Conversion and Management*, 2017, 132, 388–399.

Based on the tested performance data of three turbocharged gasoline direct injection engines, a quantitative analysis on the key influencing parameters of engine indicated thermal efficiency was focused in this study. Through excavating the inner relationships between the operational and performance parameters, a strong similarity between the indicated thermal efficiency and the effective expansion ratio was revealed. On this basis, the control equations for in-cylinder indicated thermal efficiency were corrected on the basis of ideal cycle thermal efficiency, which is changed from solely related to the compression ratio to simultaneously related to multi-parameters, including the expansion ratio, heat release rate, adiabatic efficiency, excess air coefficient, etc. In this way, a direct or indirect quantitative relation between the indicated thermal efficiency and the key influencing parameters of engine was established. The comparison results between the predicted and measured data demonstrate that the corrected control equation for engine indicated thermal efficiency can predict the influences of various parameters more accurately, and the consistency of predicted results between different engines is also satisfactory. Finally, the influence factors of engine heat-work conversion efficiency were disintegrated and the quantitative analysis was made. By this means, the influence mechanisms of key parameters on the engine heat-work conversion efficiency were revealed under various operating conditions.

Hybrid engine systems

18/00335 A review of compressed-air hybrid technology in vehicle system

Wasbari, F. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 935–953.

The aim of this paper is to present a comprehensive review of the compressed-air hybrid technology in a passenger and commercial vehicle since the beginning of its discovery to date. Hybrid technology has become popular in the automotive industry since the technology proven to improve the vehicle efficiency, saving in fuel use and green environmental. The well-known hybrid technology is hybrid electric. Nevertheless, the price of the hybrid electric automobile is high, the arrangement is complex, and it is not completely green. These disadvantages have triggered innovation in a hybrid technology called compressed-air hybrid technology. The compressed-air hybrid technology uses a combination of ICE and fluid power components as a propulsion unit and compressed-air energy as a power source. The energy stored in the tank/accumulator. Once the energy in the storage is low, the system utilizes energy losses in braking and recovers into useful energy. This article concentrates on the hybrid compressed-air design, components, latest finding, technology breakthrough, benefit and drawback of the system. The review also encompasses the most recent prototype that has been tested. Based on the study, the literature has shown that the compressed-air hybrid system is proven to work. Nevertheless, further research needs to extend out to resolve a few topics such as amending the energy capability and lightweight system design. The two-subsystem are promising, but nevertheless far from the point of commercialization. However, the three-subsystem has been proven in saving energy and fuel consumption. Although it still needs to be further refined, it has a huge potential to get into the market. The compressed-air hybrid technology in a passenger car is still new. There is a huge room to explore. If the hybrid compressed-air technology is successful, clearly it will benefit the future in the aspect of energy efficiency, cost saving, and reduce the pollution.

18/00336 Adoption barriers for electric vehicles: experiences from early adopters in Sweden

Vassileva, I. and Campillo, J. *Energy*, 2017, 120, 632–641.

Electric vehicles are considered as one of the most effective technologies for reducing current greenhouse gas emissions from the transport sector. Although in many countries, local and national governments have introduced incentives and subsidies to facilitate the electric vehicle market penetration, in Sweden, such benefits have been limited. Results from a survey carried out among private owners of electric vehicles are presented in this paper, including the analysis of the respondents socio-demographic characteristics, reasons for choosing an electric vehicle, charging locations and driving preferences, among others. The main results characterize current electric vehicle drivers as male, well-educated, with medium-high income; electric vehicles are used mainly for private purposes and charged at home during night time. Furthermore, the paper presents an analysis of the impact of large-scale penetration of electric vehicles on existing power distribution systems. The findings presented in this paper provide important insights for assuring a sustainable large-scale penetration of electric vehicles by learning from the experiences of early adopters of the technology and by analysing the impact of different electric vehicles penetration scenarios on the power distribution grid.

18/00337 Implementation methodology of powertrain for series-hybrid military vehicles applications equipped with hybrid energy storage

Lee, S. and Kim, J. *Energy*, 2017, 120, 229–240.

This paper investigates a component-sizing method and a power-control algorithm for series-hybrid military vehicles equipped with hybrid energy storages that comprise batteries and super-capacitors. Component sizing of the powertrain is determined by the performance specification that is related to mission profiles and power-flow control methods. In order to minimize the effects of mission profiles and power-flow control methods, the linear programming (LP) technique is employed. The LP problem for minimizing the output energy from the engine under different conditions of driving cycles and capacities of the energy storage system (ESS) is solved to eliminate the effect of the power distribution. Through analysing the effects of different power and energy ratings of the ESS, the optimal values of power and energy capacities of the ESS are determined. The design approaches are extensively verified with simulations and experimental results of a reduced-scale per-unit equivalent system of the 10-ton series-hybrid electric vehicle (SHEV).

18/00338 Investigating the reactivity controlled compression ignition (RCCI) combustion strategy in a natural gas/diesel fueled engine with a pre-chamber

Salahi, M. M. *et al. Energy Conversion and Management*, 2017, 132, 40–53.

Reactivity controlled compression ignition (RCCI) concept has been proven to be a promising combustion mode for the next generations of internal combustion engines. This strategy is still subject of extensive studies to overcome its operational limitations. In the present work, the effect of using a pre-chamber to extend some operating ranges in a RCCI engine is investigated using coupled multidimensional computational fluid dynamics (CFD) with detailed chemical kinetic mechanisms. To accomplish this, the combustion and flow field in a single-cylinder engine with a pre-chamber, working in RCCI mode and fuelled with natural gas/diesel are numerically modelled. Experimental data is used to validate the simulation results and then, combustion characteristics and engine emissions in some various operating regions, in terms of initial temperature, fuel equivalence ratio and portions of the two fuels are discussed. The results reveal that the proposed strategy provides the ability to extend the engine operating ranges to use lower intake temperatures, even to 50 K lower for some cases, and also using a larger portion of natural gas instead of diesel fuel. On the other hand, the new strategy could result in incomplete combustion and formation of related emissions in low loads, but for higher engine loads it shows better combustion characteristics.

18/00339 Planning of electric vehicle infrastructure based on charging reliability and quality of service

Davidov, S. and Pantoš, M. *Energy*, 2017, 118, 1156–1167.

This paper presents an optimization model for charging station placement in order to minimize the overall cost by satisfying the charging reliability and quality of service expected by electric vehicle owners/drivers. To better understand and illustrate the problem's complexity, set modelling is used to represent the road network and the electric vehicle driving trajectories. By involving the Euclidean distance, this optimization model also considers the charging reliability as well as the driving range limitation of electric vehicles. The disposable charging time of electric vehicle owners/drivers is reflected by incorporating the new quality of service index. The numeric results illustrate the application of the proposed optimization in achieving the minimal cost of charging station locations while also achieving both charging reliability and expected quality of service through the analysis of electric vehicle owners'/drivers' behaviour.

18/00340 Using detailed chemical kinetics 3D-CFD model to investigate combustion phase of a CNG-HCCI engine according to control strategy requirements

Yousefzadeh, A. and Jahanian, O. *Energy Conversion and Management*, 2017, 133, 524–534.

The homogeneous charge compression ignition (HCCI) method reduces soot and NO_x emissions by offering a high thermal efficiency in diesel engines. However, controlling HCCI combustion phenomena is known as a significant setback for its further development. Control-oriented models use CA5, CA10, CA50 and CA90 as the most important dependent variables. Start of combustion (SOC), for instance, has already been traced via pressure rise versus crank angle. In fact, these simplifications have been progressed to reach real-time response as the main nature of controlling target. In this study, a three-dimensional (3D) computational fluid dynamics (CFD) model coupled with detailed chemical kinetics has been modified to devise a brief relation between these controlling parameters and what really happens in combustion chamber. The model has been validated with experimental results in four distinct conditions. To detect combustion phase, hydroxyl radical (OH) has been suggested as an indicator among all other chemical species due to its significant role in compressed natural gas (CNG) combustion. Various sets of simulations have come up with noticeable findings that CA50 in a CNG-fuelled HCCI engine equals crank angles when OH concentration and pressure rise rate reach their peaks. This result represents OH as a potential robust parameter in HCCI engine control even though this relation is not established well in weak combustion region rather than high heat release rate (*HHR*) cases. Finally, IMEP and BSFC, as the most important performance parameters of an engine have studied versus CA50 and OH concentration variation. The comparison proved good agreement between these two terms except in near-TDC combustion cases.

Transport battery development

18/00341 A lead-acid battery's remaining useful life prediction by using electrochemical model in the particle filtering framework

Lyu, C. *et al. Energy*, 2017, 120, 975–984.

Accurate prediction of battery's remaining useful life (RUL) is significant for the reliability and the cost of systems. This paper presents a new particle filter (PF) framework for a lead-acid battery's RUL prediction by incorporating the battery's electrochemical model. An electrochemical model that simulates the charging and discharging of lead-acid battery is introduced. The effectiveness of both the model and parameter identification is validated through both synthetic and experimental data. In the new PF framework, model parameters that reflect the degradation of battery are seen as state variables, the procedure of capacity simulation and the fitting equations of known state variables are measurement model and process model respectively. Aging experiment is depicted and applied to validate the effectiveness of the method. RUL predictions are made with two different beginning points, the results of which show that the new electrochemical-model-based PF has better state variable stability and prediction accuracy than the traditional data-driven PF.

18/00342 A reliable sealing method for microbatteries

Wang, Y. *et al. Journal of Power Sources*, 2017, 341, 443–447.

As electronic devices continue to become smaller, their energy sources (i.e. batteries) also need to be smaller. Typically, energy densities of batteries decrease as the battery size decreases due to the relative increase of parasitic weight such as packaging materials. In addition, the sealing methods in conventional batteries are difficult to apply to microbatteries. This work develops a facile sealing method for microbatteries. The method employs a dual-sealing concept: a first rubber barrier temporally confines the organic electrolytes and a second adhesive barrier forms a hermetic seal with the battery case. With this innovative sealing approach, excellent shelf life and operation life of the batteries have been demonstrated. A minimal amount of packing materials is employed resulting in high energy densities.

18/00343 A two layer electrode structure for improved Li Ion diffusion and volumetric capacity in Li Ion batteries

Huang, C. *et al. Nano Energy*, 2017, 31, 377–385.

Nanomaterials with different morphologies were placed in discrete layers through the thickness of a negative electrode for a Li ion battery to exploit effectively the intrinsic energy storage capabilities of each nanomaterial morphology and to improve the overall dynamics of Li ion diffusion. The two layer electrode showed a combination of high volumetric capacity and rate capability that surpassed the performance of conventional randomly blended electrodes comprising the same nanomaterials. Local Li ion concentrations were measured through the electrode thickness and clearly showed the benefits of the layered structure over the alternatives. The two layer electrode was fabricated by a flexible and scalable suspension atomization and spray deposition technique with generic potential for improved layered electrodes in a wide range of applications.

18/00344 Battery sizing and rule-based operation of grid-connected photovoltaic-battery system: a case study in Sweden

Zhang, Y. *et al. Energy Conversion and Management*, 2017, 133, 249–263.

The optimal components design for grid-connected photovoltaic–battery systems should be determined with consideration of system operation. This study proposes a method to simultaneously optimize the battery capacity and rule-based operation strategy. The investigated photovoltaic–battery system is modelled using single diode photovoltaic model and improved Shepherd battery model. Three rule-based operation strategies – including the conventional operation strategy, the dynamic price load shifting strategy, and the hybrid operation strategy – are designed and evaluated. The rule-based operation strategies introduce different operation parameters to run the system operation. multi-objective genetic algorithm is employed to optimize the decisional variables, including battery capacity and operation parameters, towards maximizing the system's self-sufficiency ratio and net present value. The results indicate that employing battery with the conventional operation strategy is not profitable, although it increases self-sufficiency ratio. The dynamic price load shifting strategy has similar performance with the conventional operation strategy because the electricity price variation is not large enough. The proposed hybrid operation strategy outperforms other investigated strategies. When the battery capacity is lower than 72 kW h, self-sufficiency ratio and net present value increase simultaneously with the battery capacity.

18/00345 Confined selenium within metal-organic frameworks derived porous carbon microcubes as cathode for rechargeable lithium–selenium batteries

Liu, T. *et al. Journal of Power Sources*, 2017, 341, 53–59.

Unique hierarchically porous carbon microcubes (CMCs) consists of irregular bubbles derived from metal organic frameworks (MOFs) have been prepared via simple hydrothermal synthesis method and carbonization treatment. Selenium nanoparticles are uniformly dispersed in the hierarchical porous structure of CMCs by a typical melt-diffusion process, and the yielding Se/CMCs composite is enabled as a cathode material for lithium-selenium rechargeable batteries. In the carbonate-based electrolyte, with Se loading of nearly ~50 wt%, the Se/CMCs composite exhibits an ultrahigh initial discharge specific capacity of 780.4 mAh g^{-1} and still retains a reversible capacity of 425.2 mAh g^{-1} after 100 cycles at 0.2 C. Specially, these hollow structure CMCs with high conductivity contribute to the outstanding electrochemical properties by effectively decreasing the charge transfer resistance and suppressing polyselenides dissolution in carbonate electrolyte.

18/00346 Electrochemical modelling of Li-ion battery pack with constant voltage cycling

Ashwin, T. R. *et al. Journal of Power Sources*, 2017, 341, 327–339.

In a battery pack, cell-to-cell chemical variation, or the variation in operating conditions, can possibly lead to current imbalance which can accelerate pack ageing. In this paper, the pseudo-two-dimensional (P2D) porous electrode model is extended to a battery pack layout, to predict the overall behaviour and the cell-to-cell variation under constant voltage charging and discharging. The algorithm used in this model offers the flexibility in extending the layout to any number of cells in a pack, which can be of different capacities, chemical characteristics and physical dimensions. The coupled electro-thermal effects such as differential cell ageing, temperature variation, porosity change and their effects on the performance of the pack, can be predicted using this modelling algorithm. The pack charging voltage is found to have an impact on the performance as well as the SEI layer growth. Numerical studies are conducted by keeping the cells at different thermal conditions and the results show the necessity to increase the heat transfer coefficient to cool the pack, compared to single cell. The results show that the thermal imbalance has more impact than the change in inter-connecting resistance on the split current distribution, which accelerates the irreversible porous filling and ageing.

18/00347 Fe_3N constrained inside C nanocages as an anode for Li-ion batteries through post-synthesis nitridation

Huang, H. *et al. Nano Energy*, 2017, 31, 74–83.

Carbon-constraint Fe_3N nanoparticles (Fe_3N@C) with a unique core-shell structure are successfully realized through a facile two-step process: fabricating Fe@C core-shell nanoparticles by DC arc-discharge method and subsequently converting them into Fe_3N@C through chemical nitriding reactions. A series of technological conditions are carried out to manipulate the core components and the shell structure. Owing to the protection of carbon shell, the nanoparticles own clear morphology and fine dispersion without distinct sintering. The Fe_3N@C nanoparticles are applied as the anode material for lithium-ion batteries and exhibit high electric capacity in long-term cyclic charge/discharge process. Their excellent performance comes from the electrochemical lithiation/delithiation reactivity of the Fe_3N core, while stable nanostructure of the electrodes sustained in the long cycles benefits from the constraint of carbon shell mostly.

18/00348 High capacity of lithium-sulfur batteries at low electrolyte/sulfur ratio enabled by an organosulfide containing electrolyte

Chen, S. *et al. Nano Energy*, 2017, 31, 418–423.

The lithium-sulfur (Li-S) battery is a promising energy storage technology to replace lithium ion batteries for higher energy density and lower cost. Dissolution of lithium polysulfide intermediates in conventional Li-S electrolytes is known as one of the key technical barriers to the development of Li-S, because it promotes redistribution and irreversible deposition of Li_2S, and also forces large amounts of electrolyte to be used, shortening cycling life and driving down cell energy density. Recently, dimethyl disulfide as a functional co-solvent has been demonstrated to show an alternate electrochemical reaction pathway for sulfur cathodes by the formation of dimethyl polysulfides and lithium organosulfides as intermediates and reduction products. In this work, comprehensive studies show that this new pathway not only provides high capacity but also enables excellent capacity retention through a built-in automatic discharge shutoff mechanism by tuning carbon/sulfur ratio in sulfur cathodes to reduce unfavourable Li_2S formation. Furthermore, this new electrolyte system is also found to enable high capacity of high-sulfur-loading cathodes with low electrolyte/sulfur (E/S) ratios, such as a stable specific capacity of around 1000 mAh g^{-1} using a low electrolyte amount (i.e. E/S ratio of

5 mL g^{-1}) and high-sulfur-loading (4 mg cm^{-2}) cathodes. This electrolyte system almost doubles the capacity obtained with conventional electrolytes under the same harsh conditions. These results highlight the practical potential of this electrolyte system to enable high-energy-density Li-S batteries.

18/00349 Influence analysis of static and dynamic fast-charging current profiles on ageing performance of commercial lithium-ion batteries

Abdel-Monem, M. *et al. Energy*, 2017, 120, 179–191.

The rate and shape of the charging current indubitably affect the charging time and the ageing rate of a battery. Depending on the application requirements, it is possible to use high-charging current in order to decrease the charging time. However, the influence of fast-charging current profiles should be investigated to identify their impact on battery functionality over time. In this article, static and dynamic fast-charging current profiles are applied to a high power 7 Ah $LiFePO_4$-based cells, and the results of cycle-life and characterization tests are discussed. To select the proper fast-charging profile, the evaluation relies on some factors: discharge capacity retention, charging capacity, charging time, and cell temperature. After 1700 cycles, the results revealed that the dynamic fast-charging current profile has a prominent role in decreasing the degradation rate as well as the charging time of cells compared with the static fast-charging profile.

18/00350 Optimal charging for general equivalent electrical battery model, and battery life management

Abdollahi, A. *et al. Journal of Energy Storage*, 2017, 9, 47–58.

The contributions of this paper are threefold. First, the linear quadratic solution to optimally charge a Li-ion battery in a general form is presented. Although the battery model considered here is a circuit comprised of an open-circuit voltage (OCV), a series resistance, and an RC circuit, the methodology is applicable to any electrical circuit model of a battery. A combination of different cost functions is considered including: time-to-charge, energy loss, and temperature rise index. The authors discuss the effect of different weightings in the cost functions on the current and voltage profiles. Second, two models for normalized battery capacity are presented as a function of the number of cycles and two charge control parameters, namely, maximum terminal voltage of the battery and maximum charge current. These models are compared to a bi-exponential capacity model. The effectiveness of the proposed models for forecasting the battery capacity is validated using the experimental data. Finally, these models are used for battery life management by developing an optimal charging parameter selection method which provides the best setpoint values for the control variables to achieve a pre-specified desired 'useful cycle life' while attaining the fastest possible time-to-charge. The proposed optimal charging parameter selection method is illustrated via numerical results.

18/00351 Organically modified silica-supported ionogels electrolyte for high temperature lithium-ion batteries

Wu, F. *et al. Nano Energy*, 2017, 31, 9–18.

A new solid-state ionogel electrolyte was synthesized using a silane coupling agent (SCA) that can spontaneously form a porous network to confine an ionic liquid electrolyte (ILE). It was found that epoxy groups grafted on silica can promote the ionic dissociation of a lithium salt and ionic liquid. The ionogel with the optimal molar ratio (ILE/SCA = 0.75) exhibited excellent thermal stability, a wide redox stability window, and ionic conductivity of 1.91×10^{-3} S cm^{-1} at 30 °C, which is higher than that of the pure IL electrolyte. The developed ionogel improved the operating temperature of batteries from room temperature to at least 90 °C. Furthermore, the good compatibility of the ionogel with a $LiFePO_4$ cathode and $Li_4Ti_5O_{12}$ anode indicates that it can be used as an electrolyte for full battery systems. More importantly, the SCA was employed as an organosilica precursor to synthesize a new solid-state ionogel electrolyte. This new ionogel electrolyte with high stability and capacity represents a considerable advance in solid-state electrolytes for lithium-ion batteries.

18/00352 Rationally designed hollow precursor-derived $Zn_3V_2O_8$ nanocages as a high-performance anode material for lithium-ion batteries

Yin, Z. *et al. Nano Energy*, 2017, 31, 367–376.

Transition metal oxides have attracted much interest for their high energy density in lithium-ion batteries. However, large volume expansion during the lithiation process limits their practical applications. Hollow structures with porous shell (such as nanocages) can provide sufficient void space to accommodate the volume expansion during the lithiation/delithiation processes. Herein, the authors developed a novel two-step method to prepare $Zn_3V_2O_8$ nanocages, in which a hollow precursor first was obtained by a solvothermal method and then was calcined in air atmosphere. Importantly, it is found that the resultant $Zn_3V_2O_8$ nanocages possess impressive lithium storage performance in terms of high specific capacity, superior rate capability and excellent cycling stability. The excellent lithium storage performance is attributed to easy electrolyte permeability, shorter Li^+ and electron diffusion pathways, and effective alleviation of the volume expansion provided by the cage-like hollow structure. When coupled with commercially available $LiFePO_4$ cathode, the full cell exhibits remarkable lithium storage performance. The $Zn_3V_2O_8$ nanocages demonstrate a great potential as an anode material for high-performance lithium-ion batteries. In addition, the electrochemical reaction mechanism of the $Zn_3V_2O_8$ nanocages as an anode material was systematically investigated based on *ex-situ* X-ray diffraction, X-ray photo electron spectroscopy, and transmission electron microscopy.

18/00353 Silicon based lithium-ion battery anodes: a chronicle perspective review

Zuo, X. *et al. Nano Energy*, 2017, 31, 113–143.

Silicon has been regarded as one of the most promising next generation lithium-ion battery (LIB) anodes due to its exceptional capacity and proper working voltage. However, the dramatic volume change during lithiation/delithiation processes has caused severe detrimental consequences, leading to very poor cyclic stability. It has been one of the critical problems hampering the practical applications of the silicon based LIB anode. Extensive research has been carried out to resolve the problem since early 1990s. For the first time, the studies on the Si anode in the time frame more than two decades are summarized and discussed in this review with a novel chronicle perspective. Through this article, the evolution of the concept, fundamental scientific and technology development of the silicon LIB anode are clearly presented. It provides unique eyesight into this rapid developing field and will shed light on the future trend of the Si LIB anode research.

18/00354 Sodium-ion hybrid electrolyte battery for sustainable energy storage applications

Senthilkumar, S. T. *et al. Journal of Power Sources*, 2017, 341, 404–410.

Sustainable, safe, and low-cost energy storage systems are essential for large-scale electrical energy storage. This paper reports a sodium (Na)-ion hybrid electrolyte battery with a replaceable cathode system, which is separated from the Na metal anode by a Na superionic conducting ceramic. By using a fast Na-ion-intercalating nickel hexacyanoferrate (NiHCF) cathode along with an eco-friendly seawater catholyte, the authors demonstrate good cycling performance with an average discharge voltage of 3.4 V and capacity retention >80% over 100 cycles and >60% over 200 cycle. Remarkably, such high capacity retention is observed for both the initial as well as replaced cathodes. Moreover, a Na-metal-free hybrid electrolyte battery containing hard carbon as the anode exhibits an energy density of ~146 Wh kg^{-1} at a current density of 10 mA g^{-1}, which is comparable to that of lead-acid batteries and much higher than that of conventional aqueous Na-ion batteries. These results pave the way for further advances in sustainable energy storage technology.

18/00355 Ti^{3+}-free three-phase $Li_4Ti_5O_{12}/TiO_2$ for high-rate lithium ion batteries: capacity and conductivity enhancement by phase boundaries

Wang, S. *et al. Nano Energy*, 2017, 32, 294–301.

Ti-based nanoplates with abundant phase boundaries have been synthesized via partial lithiation reaction and optimized heat treatment. Using phase boundaries (rather than free surfaces) to keep the crystalline domains small might have significant advantages, such as improved tap density (therefore volumetric energy density) and reduced loss of live lithium to the solid electrolyte interphase (SEI) which only coats the free surfaces. As lithium ion battery anode, the obtained $Li_4Ti_5O_{12}/TiO_2$(Anatase)/TiO_2(Rutile) three-phase mixture shows a capacity of about 170 mA h g^{-1} at 4000 mA g^{-1} (fully charged in ~150 s), and undergoes more than 1000 cycles with capacity fade of only 0.02% per cycle. It also demonstrates excellent cycling stability even after 4000 cycles at 500 mA g^{-1} in a Li-matched full cell vs $LiFePO_4$ cathode in large pouch cell format, with tolerable gassing behaviour. Rather than relying on Ti^{3+} defects or excessively large surface area, the present material is prepared in fully oxidizing environment, with abundant phase boundaries as the main capacity enhancement mechanism, which simplify its industrial production.

18/00356 Ultra-long cycle life, low-cost room temperature sodium-sulfur batteries enabled by highly doped (N,S) nanoporous carbons

Qiang, Z. *et al. Nano Energy*, 2017, 32, 59–66.

Efficiency, cost and lifetime are the primary challenges for stationary energy storage with vanadium-redox flow and sodium-sulfur batteries as promising options. In particular, room temperature sodium-sulfur battery systems offer the potential for safe, simple, low-cost and high energy density storage, but the high reactivity or solubility of sodium polysulfides in common liquid electrolytes for carbonates or glycols, respectively, leads to rapid performance loss on cycling. Herein, the authors demonstrate a robust route to inhibit reactivity of the sulfides

with carbonate electrolytes (and also inhibit the diffusion of polysulfides dissolved in TEGDME) and prevent performance loss on cycling using highly doped (≈40 atom%) nanoporous carbon from low-cost raw materials infused with sulfur as the cathode. This cathode design leads to an ultra-stable room temperature sodium-sulfur battery with less than 3% decay in the discharge capacity after 8000 cycles at a high current density of 4.6 A/g. At 0.23 A/g, the discharge capacity is approximately 400 mAh/g and stable over 350 cycles. This combination of low cost and excellent cycle stability is promising for stationary, grid-level energy storage.

12 REFRACTORIES/ CERAMICS

Properties, production, applications

18/00357 Amplification of electrolyte uptake in the absorptive glass mat (AGM) separator for valve regulated lead acid (VRLA) batteries

Kumar, V. *et al. Journal of Power Sources*, 2017, 341, 19–26.

Absorptive glass mat (AGM) separators are widely used for valve regulated lead acid (VRLA) batteries due to their remarkable fibre and structural characteristics. Discharge performance and recharge effectiveness of VRLA batteries essentially rely on the distribution and saturation levels of the electrolyte within the AGM separator. The authors report an analytical model for predicting the wicking characteristics of AGM battery separators under unconfined and confined states. The model of wicking behaviour of AGM is based on Fries and Dreyer's approach that included the effect of gravity component which was neglected in classic Lucas-Washburn's model. In addition, the predictive model of wicking accounted for realistic structural characteristics of AGM via orientation averaging approach. For wicking under confined state, the structural parameters have been updated under defined level of compressive stresses based upon the constitutive equation derived for a planar network of fibres in AGM under transverse loading conditions. A comparison has been made between the theoretical models and experimental results of wicking behaviour under unconfined and confined states. Most importantly, this work highlights the questionable validity of classic Lucas-Washburn model for predicting the wicking characteristics of AGM separator over longer time duration.

18/00358 Analysis of silicon-based integrated photovoltaic–electrochemical hydrogen generation system under varying temperature and illumination

Bhatt, V. *et al. Journal of Energy Chemistry*, 2017, 26, (1), 72–80.

The last decade has witnessed tremendous research and development in the area of photo-electrolytic hydrogen generation using chemically stable nanostructured photo-cathode/anode materials. Due to intimately coupled charge separation and photo-catalytic processes, it is very difficult to optimize individual components of such system leading to a very low demonstrated solar-to-fuel efficiency (SFE) of less than 1%. Recently there has been growing interest in an integrated photovoltaic–electrochemical (PV–EC) system based on GaAs solar cells with the demonstrated SFE of 24.5% under concentrated illumination condition. But a high cost of GaAs based solar cells and recent price drop of poly-crystalline silicon (pc-Si) solar cells motivated researchers to explore silicon based integrated PV–EC system. In this paper a theoretical framework is introduced to model silicon-based integrated PV–EC device. The theoretical framework is used to analyse the coupling and kinetic losses of a silicon solar cell based integrated PV–EC water splitting system under varying temperature and illumination. The kinetic loss occurs in the range of 19.1%–27.9% and coupling loss takes place in the range of 5.45%–6.74% with respect to varying illumination in the range of 20–100 mW/cm^2. Similarly, the effect of varying temperature has severe impact on the performance of the system, wherein the coupling loss occurs in the range of 0.84%–21.51% for the temperature variation from 25 to 50 °C.

18/00359 Comparative studies of encapsulation and glass surface modification impacts on PV performance in a desert climate

Walwil, H. M. *et al. Solar Energy*, 2017, 142, 288–298.

Photovoltaic (PV) module encapsulation and glass covering processes play big role in reliability and performance of PV modules, especially under desert climatic conditions. In the present study, tests were carried out to compare the performance of five types of commercial glass cover and three types of commercial PV module encapsulates. The relative advantages of anti-reflective coated and textured glass cover, as well as, silicone and Ionomere encapsulant under clean and dusty conditions were examined in terms of PV module's power output and temperature. The results revealed that silicone and Ionomere encapsulant do boost the power output of a clean PV module by 2–3% on average. However, ethylene-vinyl acetate (EVA) encapsulant dust-covered modules showed relatively better performance as compared to dust-covered Ionomere and silicone encapsulant modules. Clean modules encapsulated with silicone or Ionomere material exhibited higher module temperature relative to that of EVA encapsulant modules. Adding an anti-reflective coating and texturing module's surface in some cases boosted the power output of a clean PV module by 6% on average. In addition, the study confirmed the fact that dust fouling can lead to a significant reduction in PV module power output (40% reduction after 10 months of exposure without cleaning). Anti-reflective coating of PV modules glass cover can relatively mitigate power reduction due to dust coverage.

18/00360 Conversion of nuclear waste to molten glass: formation of porous amorphous alumina in a high-Al melter feed

Xu, K. *et al. Journal of Nuclear Materials*, 2017, 483, 102–106.

The transition of Al phases in a simulated high-Al high-level nuclear waste melter feed heated at 5 K min^{-1} to 700 °C was investigated with transmission electron microscopy, ^{27}Al nuclear magnetic resonance spectroscopy, the Brunauer–Emmett–Teller method and X-ray diffraction. At temperatures between 300 and 500 °C, porous amorphous alumina formed from the dehydration of gibbsite, resulting in increased specific surface area of the feed (~8 $m^2 g^{-1}$). The high-surface-area amorphous alumina formed in this manner could potentially stop salt migration in the cold cap during nuclear waste vitrification.

18/00361 Correlations for glazing properties and representation of glazing types with continuous variables for daylight and energy simulations

Gosselin, L. and Dussault, J.-M. *Solar Energy*, 2017, 141, 159–165.

In daylight and energy simulations, fenestration products are characterized by their visible transmittance (VT) and solar heat gain coefficient (SHGC) that are both dependent on the angle of incidence, as well as by their U-value. In this work, 18 typical fenestration products suitable for the Canadian context were chosen and correlations between their actual properties were developed. First, it is shown that variations from a 'standard' angular dependency curve for VT and SHGC are relatively small in such a way that the angular dependency can be approximated either by an average relation for all fenestration types, or by more precise correlations involving a linear combination of solutions with the use of a weigh coefficients. Then, relationships between values of normal VT, U-value and normal SHGC are established. In the end, it was possible to deduce the detailed behaviour of all insulated glazing units (IGU) from only one continuous variable. A more precise approach with three continuous variables was also developed. A test case is presented to illustrate how to use the correlations to generate different types of IGUs in simulations.

18/00362 Design optimization of multi-layer silicon carbide cladding for light water reactors

Lee, Y. *et al. Nuclear Engineering and Design*, 2017, 311, 213–223.

A parametric study that demonstrates a methodology for determining the optimum bilayer composition in a duplex SiC cladding is discussed. The structural performance of multi-layer SiC cladding design is significantly affected by radial thickness fraction of each layer. This study shows that there exists an optimal composite/monolith radial thickness fraction that minimizes failure probability for a duplex SiC cladding in steady-state operation. An exemplary reference case study shows that the duplex cladding with the inner composite fraction ~0.4 and the outer CVD-SiC fraction ~0.6 is found to be the optimal SiC cladding design for the current PWRs with the reference material choice for CVD-SiC and fibre reinforced composite. A marginal increase in the composite fraction from the presented optimal designs may lead to increase structural integrity by introducing some unquantified merits such as increasing damage tolerance. The major factors that affect the optimum cladding designs are temperature gradients and internal gas pressure. Clad wall thickness, thermal conductivity, and Weibull modulus are among the key design parameters/material properties.

18/00363 Effect of bismuth titanate on the properties of potassium sodium niobate-based ceramics

Mgbemere, H. E. *et al. Journal of Asian Ceramic Societies*, 2017, 5, (1), 49–55.

The effect of modifying the properties of KNN-based ceramics with $Bi_2Ti_2O_7$ (BiT) been investigated in this work. The density measurements show that additions of BiT to the samples slightly increase the

density values. Scanning electron microscope images of the samples indicate that the average sizes of the grains decrease with BiT addition while the volume of pores increase. X-ray diffraction results show that for $(K_{0.5}Na_{0.5})NbO_3$ based samples, a transformation from orthorhombic to pseudo-cubic phase is observed. For both $K_{0.48}Na_{0.48}Li_{0.04})(Nb_{0.9}Ta_{0.1})O_3$ and $K_{0.48}Na_{0.48}Li_{0.04})(Nb_{0.86}Ta_{0.1}Sb_{0.04})O_3$-based compositions, the phase transition is from an orthorhombic-tetragonal coexistence to a tetragonal structure dominated phase coexistence. The dielectric constant, dielectric loss and resistivity values of the samples increase slightly with BiT addition. Good hysteresis curves are obtained in $(K_{0.5}Na_{0.5})NbO_3$-based samples only at low BiT amounts. Remnant polarization values between 9 μC/cm^2 and 25 μC/cm^2 are obtained for $K_{0.48}Na_{0.48}Li_{0.04})(Nb_{0.9}Ta_{0.1})O_3$ and $K_{0.48}Na_{0.48}Li_{0.04})(Nb_{0.86}Ta_{0.1}Sb_{0.04})O_3$-based samples. With the exception of KNNLT samples where the d^*_{33} values increase from 203 ± 7 pm/V at 0 mol% to 275 ± 6 pm/V at 0.35 mol%, the d^*_{33} values of the samples gradually decrease with increasing BiT content. This work shows that to obtain good properties for KNN-based ceramics, only very small amounts of BiT are required.

18/00364 Experimental chiller with silica gel: adsorption kinetics analysis and performance evaluation

Vodianitskaia, P. J. *et al. Energy Conversion and Management*, 2017, 132, 172–179.

Adsorption technology is a promising, low carbon intensity option for air conditioning and refrigeration. Adsorption kinetics is a key performance factor for such systems. This paper presents an adsorption kinetics and performance assessment of an experimental adsorption chiller with silica gel and water as working pair. The adsorbent bed heat exchanger is equipped with silica gel in loose grains fitted between finned tubes. Pressure, temperature and adsorbate flow measurements along the thermodynamic cycle are performed for two different options of adsorbent particle fraction sizes to compare the resulting dynamics and performance. *COP* is 0.53 and *SCP* is 68 W kg^{-1} for 2.0 mm diameter silica gel and a 80/30/15 °C triplet. COP is 4 % worse when 0.26 mm silica gel is used, due to the lower porosity and lower thermal conductivity presented by the crushed adsorbent. A mass diffusion algorithm is considered in the numerical model. Good agreement between experimental and calculated data has been reached. The maximum temperature level needed for desorption in the 70–80 °C range is compatible with the use of water heated by flat-type solar collectors, and low-grade waste heat from industrial processes.

18/00365 Heat transfer, pressure drop and structural analysis of a finned plate ceramic heat exchanger

de Mello, P. E. B. *et al. Energy*, 2017, 120, 597–607.

High-temperature heat exchangers (HTHE) constructed with ceramics can achieve higher temperatures of operation. Resistance to oxidation is the great advantage of using ceramics for this application. This paper presents experimental characterization of one ceramic heat exchanger composed of finned plates operating at temperatures as high as 800 °C and Reynolds number between 170 and 2000. The heat exchanger operates in counter-flow with air in both sides. The plates were constructed using alumina (Al_2O_3) with the Gelcasting technique. Thermal performance was obtained in the form of Colburn and friction factors as a function of Reynolds number. The heat exchanger effectiveness varied between 0.620 and 0.901. Progressively higher temperature was imposed to the heat exchanger prototype to cause structural failure. In addition, the design and structural integrity assessments were carried out using refined finite element computations based on real experiments regarding fracture resistance of the employed ceramic. Thermal performance of the ceramic heat exchanger is adequate and predictable using CFD simulations, but guarantee structural integrity remains challenging.

18/00366 Impact of specialty glass and concrete on gamma shielding in multi-layered PWR dry casks

Waly, E.-S. A. *et al. Progress in Nuclear Energy*, 2017, 94, 64–70.

There is a strong likelihood that dry casks will be relied on for many decades to come as the storage system for nuclear spent-fuel high-level waste (HLW), which places importance on robust shielding materials for cask construction. A dry cask with multi-layered shielding has been simulated in MicroShield v9.05 to determine exposure rates due to gamma-rays at the outer cask surface. The cask consists of a 0.27 ft thick stainless steel type 303Cu waste basket, a 0.2 ft thick lead oxide glass shielding layer (named as Glass 6), and a 1.8 ft thick overpack made of a specialty high-density concrete (named as Concrete 6). Three spent fuel configurations have been used as photon sources, which include one high burnup (72 GWd/MTU) and two medium burnup (38.6 GWd/MTU) fuels. The cumulative exposure rate over all photon energies from 15 keV to 2 MeV is 6.81E-6 mR/h at the outer cask surface for the high burnup spent fuel. This is roughly one order of magnitude smaller than if the glass layer were replaced with an equivalent thickness of Concrete 6 and is three or four orders of magnitude smaller than replacing the specialty concrete with ordinary, standard density concrete. Varying the ratio of the glass thickness to the concrete thickness significantly impacts the shielding effectiveness, which should be considered along with structural and thermal stability for dry cask designs.

18/00367 Lead recovery and high silica glass powder synthesis from waste CRT funnel glasses through carbon thermal reduction enhanced glass phase separation process

Xing, M. *et al. Journal of Hazardous Materials*, 2017, 322, 479–487.

In this study, a novel process for the removal of toxic lead from the cathode ray tube (CRT) funnel glass and synchronous preparation of high silica glass powder was developed by a carbon-thermal reduction enhanced glass phase separation process. CRT funnel glass was remelted with B_2O_3 in reducing atmosphere. In the thermal process, a part of PbO contained in the funnel glass was reduced into metallic Pb and detached from the glass phase. The rest of PbO and other metal oxides (including Na_2O, K_2O, Al_2O_3, BaO and CaO) were mainly concentrated in the boric oxide phase. The metallic Pb phase and boric oxide phase were completely leached out by 5 mol/L HNO_3. The lead removal rate was 99.80% and high silica glass powder (SiO_2 purity > 95 wt%) was obtained by setting the temperature, B_2O_3 added amount and holding time at 1000 °C, 20% and 30 min, respectively. The prepared high silicate glass powders can be used as catalyst carrier, semipermeable membranes, adsorbents or be remelted into high silicate glass as an ideal substitute for quartz glass. Thus this study proposed an eco-friendly and economical process for recycling Pb-rich electronic glass waste.

18/00368 Life cycle impact assessment of photovoltaic power generation from crystalline silicon-based solar modules in Nigeria

Akinyele, D. O. *et al. Renewable Energy*, 2017, 101, 537–549.

This paper evaluates the life cycle impact (LCI) of a 1.5 kW solar photovoltaic (PV) system. The LCI is examined in terms of the life cycle emission rate (LCER), global warming potential (GWP), cumulative energy demand (CED), energy payback time (EPT) and net energy ratio (NER), using six different locations – one from each of Nigeria's six geo-political zones as case studies. With a performance ratio of 80%, lifetime of 20–30 years, module efficiency of 15.4%, solar irradiation of 1493–2223 kWh/m^2/yr, LCER of 37.3–72.2 g CO_2/kWh and CED of 3800–8700 MJ eq., the GWP, EPT and NER values of 1907–5819 kg CO_2-eq., 0.83–2.3 years and 7.08–36.17, respectively, are obtained. The significance of these results is that the lowest GWP and EPT, i.e. 1907 kg CO_2-eq. and 0.83 years, are obtained for the location with the highest solar irradiation, while the highest values, i.e. 5819 kg CO_2-eq. and 2.3 years, are obtained for the location with the lowest irradiation. Furthermore, the highest NER is obtained for the location with the highest irradiation while the lowest value has been obtained for the location having the lowest irradiation. The study provides an insight into the significance and impact of a location's solar energy potential on the environmental performance of a PV system, which can be useful for energy analysis, planning and decision-making purposes.

18/00369 Modelling aqueous corrosion of nuclear waste phosphate glass

Poluektov, P. P. *et al. Journal of Nuclear Materials*, 2017, 484, 357–366.

A model is presented on nuclear sodium alumina phosphate (NAP) glass aqueous corrosion accounting for dissolution of radioactive glass and formation of corrosion products surface layer on the glass contacting ground water of a disposal environment. Modelling is used to process available experimental data demonstrating the generic inhibiting role of corrosion products on the NAP glass surface.

18/00370 Natural halloysite nano-clay electrolyte for advanced all-solid-state lithium-sulfur batteries

Lin, Y. *et al. Nano Energy*, 2017, 31, 478–485.

Solid polymer electrolytes (SPEs) show increasing potential for application in high energy lithium sulfur batteries due to good flexibility and high safety. However, low room temperature ionic conductivity of SPEs has become the main limitation. Herein, a novel SPE film using natural halloysite nano-clay has been fabricated, which exhibits exceptional ionic conductivity of 1.11×10^{-4} S cm^{-1} and lithium ion transference number of 0.40 at 25 °C. The mechanism of enhanced lithium ion transport is considered. The oppositely charged halloysite nanotube surfaces separate lithium salt into lithium ions that are absorbed on the negatively charged outer silica surface, and anions may be accommodated on the positively charged inner aluminol surface. So, an ordered 3D structure for free lithium ion transport is suggested. This potential application of the natural halloysite nano-clay has been demonstrated by an all-solid-state lithium-sulfur battery over a wide temperature range of 25–100 °C. These results reveal the possibility of realizing sustainable high energy storage at a reduced cost.

18/00371 Optical, spectral and thermal properties of natural pumice glass

Correcher, V. *et al. Radiation Physics and Chemistry*, 2017, 130, 69–75.
Pumice is a natural Si-rich material displaying a complex cathodoluminescence (CL) and thermoluminescence (TL) glow curves. The UV-IR CL emission consists of (i) a UV waveband in the range of 340–420 nm, (ii) blue band at 450–480 nm and (iii) a broad emission in the green-red region (at 550–650 nm) that could be respectively linked to non-bridging oxygen hole centres (≡Si–O·), self-trapped excitons and point defects (Mn^{2+} ~0.03% and Fe ~1.15%). Thermal treatments performed on the TL glow curves allowed us to determine that the trap system could be associated with a continuum in the trap distribution, since successive thermal pretreatments in the range of 200–310 °C induce an emission that shifts linearly to higher temperatures when the thermal pretreatment (T_{stop}) is increased, while the intensity of the maxima decreases similarly to the peak area. The evaluation of the E_a values, *s* value and the trap system calculated by VHR, IR and glow curve fitting methods considering three possible distribution function for $n(E)$: Gaussian, exponential and uniform, has given matching values for the 280 °C TL peak.

18/00372 Phase stability, swelling, microstructure and strength of Ti_3SiC_2-TiC ceramics after low dose neutron irradiation

Ang, C. *et al. Journal of Nuclear Materials*, 2017, 483, 44–53.
$M_{n+1}AX_n$ (MAX) phase Ti_3SiC_2 materials were neutron irradiated at ~400, ~630 and 700 °C to a fluence of $\sim 2 \times 10^{25}$ n/m^2 (E > 0.1 MeV). After irradiation at ~400 °C, anisotropic c-axis dilation of ~1.5% was observed. Room temperature strength was reduced from 445 ± 29 MPa to 315 ± 33 MPa and the fracture surfaces showed flat facets and transgranular cracks instead of typical kink-band deformation and bridging ligaments. XRD phase analysis indicated an increase of 10–15 wt% TiC. After irradiation at ~700 °C there were no lattice parameter changes, ~5 wt% decomposition to TiC occurred, and strength was 391 ± 71 MPa and 378 ± 31 MPa. The fracture surfaces indicated kink-band based deformation but with lesser extent of delamination than as-received samples. Ti_3SiC_2 appears to be radiation tolerant at ~400 °C, and increasingly radiation resistant at ~630–700 °C, but a higher temperature may be necessary for full recovery.

18/00373 Potential of producing solar grade silicon nanoparticles from selected agro-wastes: a review

Adebisi, J. A. *et al. Solar Energy*, 2017, 142, 68–86.
The US Energy Information Administration (EIA) stated that Nigeria generates around 3080 MW of electricity but with actual estimated demand of 10,000 MW. Due to the low electricity generation, total energy consumption profile of Nigeria showed that about 99% of the energy consumed is derived from fossil fuels which invariably contribute to greenhouse gases emission. Electricity, if readily available at low cost, can easily replace the fossil fuels which pose adverse effect on the citizen and climate. Solar photovoltaic is identified as an effective renewable energy source that has proven to be a promising candidate for provision of clean and sustainable electricity. Silicon is the leading commercialized terrestrial PV material for making solar cell due to its relative efficiency. This review work highlights the viability of using abundant agricultural wastes in Nigeria to produce nano-sized solar grade silicon employing methods that will require less energy. Details of previous silicon (nanoparticles) synthesized from agricultural wastes are dissected. Production of silicon nanoparticles from this origin could provide low cost solar grade silicon compared with high temperature robust methods currently been used to obtain them. Hence various methods of producing nanoparticles are highlighted.

18/00374 Scintillation and luminescence characteristics of Ce^{3+} doped in Li_2O–Gd_2O_3–BaO–B_2O_3 scintillating glasses

Zaman, F. *et al. Radiation Physics and Chemistry*, 2017, 130, 158–163.
Ce^{3+} activated Li_2O–Gd_2O_3–BaO–B_2O_3 glass scintillator containing neutron-capture elements (^{7}Li, ^{11}Band ^{158}Gd) were developed by conventional melt-quenching technique. Luminescence spectra under UV and X-ray excitation showed Ce^{3+}ion emission due to 5d → 4f transition at 391 nm. Energy transfer from the host glass to Ce^{3+}ions were confirmed by VUV–UV and XEL spectra. The highest emission intensity of Ce^{3+}ions were observed at 0.5 mol% of CeF_3. For the same concentration the decay time was obtained to be 19.7 ns and their mean critical distance was calculated about 22.33 Å. The observed decay constants revealed that direct electron-hole capture was a dominant scintillation process in the present glass matrix.

18/00375 Simultaneously enhanced toughness and strain tolerance of SiC-based ceramic composite by in-situ formation of VB_2 particles

Li, Y. *et al. Journal of the European Ceramic Society*, 2017, 37, (1), 399–405.
SiC-30vol%VB_2 ceramic composite was prepared by pressureless densification at 2150 °C with excess B_4C and C as sintering aids after *in situ* formation of VB_2 in SiC matrix. The sintered bulk gained a considerably high fracture toughness of 7.0 ± 0.4 MPa m$^{1/2}$, which was ~2.4 times as high as that of the monolithic SiC ceramic, owing to the existences of weak heterophase boundaries, thermal residual stresses and microcracks. Meanwhile, since the VB_2 particle has a lower elastic modulus than SiC and significantly suppressed the grain growth of SiC, the composite exhibited a high flexural strength of 458 ± 36 MPa and a relatively low Young's modulus of 356 ± 6 GPa, resulting in an increase of ~59.3% in mechanical strain tolerance (1.29×10^{-3}) compared with that of single-phase SiC ceramic. Besides, the residual stresses and microcracks also induced a lower-than-expected Vickers hardness of 20.8 ± 0.5 GPa in the composite.

18/00376 Sodium–aluminum–iron phosphate glasses as legacy high level waste forms

Stefanovsky, S. V. *et al. Progress in Nuclear Energy*, 2017, 94, 229–234.
Legacy liquid high level wastes (HLW) generated at former defence programmes, which are under storage in stainless steel tanks at PA Mayak have high Fe/Al contents. They will be vitrified in a new EP-500 J-heated ceramic melter, which is planned to be commissioned in 2016. Like previous melters of the same type, the new melter will produce aluminophosphate based glass. Due to high content of iron oxides in the HLW the glass obtained will have base sodium–aluminium–iron phosphate composition. Complex sodium–aluminium–iron phosphate glassy materials with various Al_2O_3 to Fe_2O_3 ratio containing high level waste (HLW) surrogate were designed, produced, and characterized by X-ray diffraction and scanning electron microscopy. The samples were annealed by a canister centreline cooling regime at the EP-500 plant. Addition of B_2O_3 and partial Fe_2O_3 substitution for Al_2O_3 in the materials increases resistance to devitrification whereas further substitution and NiO incorporation increase significantly tendency to devitrification. All the glasses had low leachability satisfying to Russian standard R 52126-2003 (similar to MCC-1 at 25 °C) but the glasses at Al_2O_3:Fe_2O_3 ratio close to 1 were found to be the highest chemically durable.

18/00377 Structural analysis of mixed alkali borosilicate glasses containing Cs^+ and Na^+ using strong magnetic field magic angle spinning nuclear magnetic resonance

Kaneko, S. *et al. Journal of Asian Ceramic Societies*, 2017, 5, (1), 7–12.
The authors have investigated the local structure of alkali atoms in mixed alkali silicate, borate, and borosilicate glasses, which contain Cs^+ and Na^+, using strong magnetic field magic angle spinning nuclear magnetic resonance (MAS NMR) spectroscopy of ^{133}Cs and ^{23}Na. The spectral peaks of ^{133}Cs in borosilicate (Si : B = 1 : 1) and Si-rich borosilicate (Si : B = 2 : 1) glasses shifted to upfield with increasing $Cs^+/(Na^+ + Cs^+)$ ratio, which implies that the coordination number of Cs^+ decreased as in the case of silicate and borate glasses. However, this trend was not observed in the ^{23}Na spectra of either borosilicate glass. This might be because the chemical shift of ^{23}Na in borosilicate glass is strongly affected by nearby species such as Si or B, and not by the coordination number of Na^+.

18/00378 Surface reliability of annealed and tempered solar protective glasses: indentation and scratch behavior

Humood, M. *et al. Solar Energy*, 2017, 142, 13–25.
Solar glass is exposed to mechanical contact cleaning and sand particle impact during operation in outdoor environments resulting in optical efficiency loss as well as decrease in mechanical integrity, durability and reliability. The current study investigates the mechanical behaviour of two different solar surface glasses through a series of low and high load indentation and scratch experiments. Nanoindentation experiments are performed on the glass substrate in order to measure the hardness and elasticity moduli at different depths below the surface. Scratch experiments are also preformed to find the critical load for the extent of plastic zone or the onset of micro-cracking. The influence of heat treatment for photovoltaic glasses on mechanical properties such as elastic modulus and hardness, and surface properties such as friction coefficient and elastic recovery is examined in this study in which heat treatment is found to affect both mechanical and surface properties. Also, different resistance behaviour is observed in low and high load experiments as well as in indentation vs scratch experiments.

18/00379 Thermal conductivity analysis of SiC ceramics and fully ceramic microencapsulated fuel composites

Lee, H.-G. *et al. Nuclear Engineering and Design*, 2017, 311, 9–15.
The thermal conductivity of SiC ceramics and FCM fuel composites, consisting of a SiC matrix and TRISO coated particles, was measured and analysed. SiC ceramics and FCM pellets were fabricated by hot press sintering with Al_2O_3 and Y_2O_3 sintering additives. Several factors that influence thermal conductivity, specifically the content of sintering additives for SiC ceramics and the volume fraction of TRISO particles and the matrix thermal conductivity of FCM pellets, were investigated.

The thermal conductivity values of samples were analysed on the basis of their microstructure and the arrangement of TRISO particles. The thermal conductivity of the FCM pellets was compared to that predicted by the Maxwell-Eucken equation and the thermal conductivity of TRISO coated particles was calculated. The thermal conductivity of FCM pellets in various sintering conditions was in close agreement to that predicted by the Maxwell–Eucken equation with the fitted thermal conductivity value of TRISO particles.

18/00380 Thermoelectric heat recovery from glass melt processes

Yazawa, K. *et al. Energy*, 2017, 118, 1035–1043.

Thermoelectric energy recovery from waste heat in glass melting process is investigated without any detrimental design or process changes. Melting glass pellets require a furnace with temperature over 1500 °C for downstream glass shaping processes and hence a large amount of exergy is available but currently destroyed. Due to high temperature gradients, parasitic losses are investigated in conjunction with the optimum thermoelectric design for maximum power output and the lowest cost. Among variations of thermal paths, the fireports are identified as the best potential for lowest cost. By partially replacing the refractory wall in thickness with a thermoelectric generator, heat loss is kept at the current 9 kW/m^2. High temperature gradients across the thermoelectric generator requires a water cooling heat sink. The cost of the heat sink is included in the overall energy and cost analysis. Based on a typical thermoelectric figure-of-merit ($ZT = 1$), optimally designed thermoelectric integrated system generates 55.6 kW of electricity with efficiency of over 15% from a 500 ton/day (5.8 kg/s) scale glass production at an additional cost of $1–2/W. This technology can provide 1.37 billion kWh of primary energy savings annually, if it is implemented throughout the whole glass industry in the USA.

18/00381 Ultra-high elevated temperature strength of TiB_2-based ceramics consolidated by spark plasma sintering

Demirskyi, D. *et al. Journal of the European Ceramic Society*, 2017, 37, (1), 393–397.

Spark plasma sintering of TiB_2–boron ceramics using commercially available raw powders is reported. The B_4C phase developed during reaction-driven consolidation at 1900 °C. The newly formed grains were located at the grain junctions and the triple point of TiB_2 grains, forming a covalent and stiff skeleton of B_4C. The flexural strength of the TiB_2–10 wt% boron ceramic composites reached 910 MPa at room temperature and 1105 MPa at 1600 °C. Which is the highest strength reported for non-oxide ceramics at 1600 °C. This was followed by a rapid decrease at 1800 °C to 480–620 MPa, which was confirmed by increased number of cavitated titanium diboride grains observed after flexural strength tests.

18/00382 Variation of energy absorption and exposure buildup factors with incident photon energy and penetration depth for boro-tellurite (B_2O_3-TeO_2) glasses

Sayyed, M. I. and Elhouichet, H. *Radiation Physics and Chemistry*, 2017, 130, 335–342.

The gamma-ray energy absorption (EABF) and exposure buildup factors (EBF) of $(100–x)TeO_2–xB_2O_3$ glass systems (where x = 5, 10, 15, 20, 22.5 and 25 mol%) have been calculated in the energy region 0.015–15 MeV up to a penetration depth of 40 mfp (mean free path). The five parameters (G–P) fitting method has been used to estimate both EABF and EBF values. Variations of EABF and EBF with incident photon energy and penetration depth have been studied. It was found that EABF and EBF values were higher in the intermediate energy region, for all the glass systems. Furthermore, boro-tellurite glass with 5 mol% B_2O_3, was found to present the lowest EABF and EBF values, hence it is superior gamma-ray shielding material. The results indicate that the boro-tellurite glasses can be used as radiation shielding materials.

13 ALTERNATIVE ENERGY SUPPLIES

Biofuels and bioconversion energy

18/00383 A review and future directions in techno-economic modeling and optimization of upstream forest biomass to bio-oil supply chains

Mirkouei, A. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 15–35.

Recent interest in biomass supply chain management has stimulated research efforts in the industry and academic communities. Techno-economic modelling and optimization efforts targeted on the upstream segment of the forest biomass to bio-oil supply chain are reviewed. Key components of upstream supply chain decision making are then presented through an overview and classification of the existing methods and contributions. There is a need to classify and analyse the relevant methodologies and approaches identified in prior studies, and to subsequently assess their usefulness through empirical research and case-based analysis. Both narrative and systematic literature reviews are performed using qualitative analysis and classic bibliometric techniques to demonstrate the scope of current papers and the call for future needs. It is found, due to growing demands for bioenergy, future biomass-to-bioenergy supply chains should draw upon existing research toward the development of efficient and effective forest biomass supply chain networks. It is further concluded that a new generation of pre-treatment technologies is needed for techno-economic optimization of upstream forest biomass value chains.

18/00384 Biodiesel production by lipase-catalyzed transesterification of *Ocimum basilicum* L. (sweet basil) seed oil

Amini, Z. *et al. Energy Conversion and Management*, 2017, 132, 82–90.

The increasing global demand for fuel, limited fossil fuel resources, and increasing concern about the upturn in gaseous CO_2 emissions are the key drivers of research and development into sources of renewable liquid transport fuels, such as biodiesel. This work demonstrates biodiesel production from *Ocimum basilicum* (sweet basil) seed oil by lipase-catalysed transesterification. Sweet basil seeds contain 22% oil on a dry weight basis. Artificial neural network with genetic algorithm modelling was used to optimize reaction. Temperature, catalyst concentration, time, and methanol to oil molar ratio were the input factors in the optimization study, while fatty acid methyl ester (FAME) yield was the key model output. FAME composition was determined by gas chromatography mass spectrometry. The optimized transesterification process resulted in a 94.58% FAME yield after reaction at 47 °C for 68 h in the presence of 6% w/w catalyst and a methanol to oil ratio of 10 : 1. The viscosity, density, calorific value, pour point, and cloud point of the biodiesel derived from sweet basil seed oil conformed to the EN 14214 and ASTM D6751 standard specifications. The antioxidant stability of the biodiesel did not meet these specifications but could be improved via the addition of antioxidant.

18/00385 Biomass and nutrient mass of *Acacia dealbata* and *Eucalyptus globulus* bioenergy plantations

Albaugh, T. J. *et al. Biomass and Bioenergy*, 2017, 97, 162–171.

In this study, the authors quantified biomass and nutrient accumulation of *Acacia dealbata* Link and *Eucalyptus globulus* Labill. planted at stem densities of 5000 and 15,000 ha^{-1} in a bioenergy plantation in Chile. They tested the hypotheses that species and stocking will not affect biomass or nutrient accumulation. Species and stocking did not affect biomass accumulation after 5 years; however, species and stocking did influence nutrient mass. *A. dealbata* had higher nitrogen mass than *E. globulus* for total (397 kg ha^{-1} more, i.e. 126% higher), foliage (188 kg ha^{-1}, 218%), branch (55 kg ha^{-1}, 95%), stem (120 kg ha^{-1}, 86%) and root (34 kg ha^{-1}, 109%) components, likely because *A. dealbata* fixes nitrogen. *A. dealbata* had lower calcium mass than *E. globulus* for branch (111 kg ha^{-1}, 60%) and stem (69 kg ha^{-1}, 39%) components. Root nitrogen and phosphorus masses and foliage, branch and root boron masses were significantly lower with a stocking density of 5000 ha^{-1}. Low stocking produced the same amount of total biomass as high stocking for both species and would be less expensive to plant. *A. dealbata* had higher nitrogen mass and likely increased soil nitrogen. *E. globulus* had high calcium mass in the stem and branches; off-site losses could be mitigated with stem-only harvests and debarking of stems in the field. Given the rainfall patterns and water availability constraints in Chile, additional criteria including water use efficiency would be required to determine the best species for bioenergy plantations in Chile.

18/00386 Biomass conservation using an optimised drying process for energy sorghum bagasse

Iqbal, T. *et al. Renewable Energy Focus*, 2017, 19–20, 1–7.

Sorghum bagasse in recent years has emerged as a promising feedstock for production of biofuels and value-added products following various biological conversion pathways. However, adequate conservation is critical for utilizing sorghum bagasse as a feedstock for fuel production around the year in bioenergy plants. Therefore, this study aims to examine the pressure drop as a function of airflow velocity and construct Shedd's curves for energy sorghum bagasse. The ambition was to facilitate large-scale drying systems for biomass conservation. The bagasse was prepared by extracting the juice from the harvested sorghum and passing through a juicing machine. Afterwards, it was manually chopped and stored on a wooden platform having 2.44 m^2 area in a 55-gallon drum at a depth of 0.57 m. The airflow velocities (0.24–1.32 ms^{-1}) caused a pressure drop (9.96–346.23 Pa) across the empty drum. The different pressure drop in the drum containing sorghum bagasse (19.92–263.25 Pa) was due to various airflow velocities (0.043–0.799 ms^{-1}). Pressure drop was further increased with increasing airflow velocity, and it was found in line with the values of pressure drop for ear and shelled corn, as reported in ASABE standards. Shedd's curves for sorghum bagasse samples were developed, as these curves can be used for designing large-scale aeration systems for chopped energy sorghum. The whole production chain of biofuel by conserving biomass can be improved by the findings of this work, thus allowing the biomass to be used more economically around the year in bioenergy plants.

18/00387 Can biomass be satisfactorily gasified under pressure using an aqueous slurry feed? Examination by simulation

Stanmore, B. and Nzihou, A. *Biomass and Bioenergy*, 2017, 97, 108–115.

A major hurdle for the gasification of biomass under pressure is the need to introduce a fibrous biomass feed material such as straw, switchgrass or Miscanthus into a pressure vessel. One proposed solution is to prepare a dense aqueous slurry from the biomass and then use a conventional high pressure pump. The production of syngas from wheat straw and subsequent power generation is examined theoretically in an Australian context. A slurry of concentration of 50% biomass by volume, which is regarded as the maximum pumpable value, is dried with superheated steam and the biomass gasified at 2 MPa with steam only in cyclones. It was found that the thermal deficiency of introducing excessive liquid water is considerable, rendering the process unsustainable. The problem can be overcome by employing a subsidiary fuel such as natural gas, but even with the minimal amount of water, the required energy input is equivalent to that of the straw. The net electrical efficiency of the process based on both fuels is 33.5%, so that the approach would be contemplated only if the overriding consideration was the use of the straw for energy generation. The zero net present value cost of power production is 125 $ MWh^{-1} for 90 Gg of straw consumption per annum.

18/00388 Characterization of biofuel refinery byproduct via selective electrospray ionization tandem mass spectrometry

Boes, K. S. *et al. Fuel*, 2017, 188, 190–196.

To achieve economic viability, biorefineries need to increase efficiency through characterization of byproducts for the purpose of valorization. One such byproduct is the liquid stream produced after autohydrolysis pre-treatment, autohydrolysate liquor, which contains valuable organic derivatives of hemicellulose and lignin from biomass. To characterize the autohydrolysis liquor, a novel method for such liquor analysis that uses electrospray ionization and ion dopants was employed in combination with tandem mass spectrometry using a quadrupole–time-of-flight mass spectrometer. Electrospray expands current analysis of such liquors through softer ionization. Ion dopants provide for differentiation of the complex mixture components without requiring derivatization or preliminary separation. The dopants – ammonium chloride and sodium hydroxide – primarily target and enhance ionization of hemicellulosic or lignin derivative species, respectively, based on the species' differing functionalities. Valuable structural information can be gleaned from these enhanced species by ion isolation and collision-activated dissociation (CAD), which reveals the presence of hemicellulosic or lignin derivative functionalities. These ionization techniques coupled with CAD enabled us to not only confirm the presence of low molecular weight ions, such as vanillin, as previously seen with gas chromatography-mass spectrometry but also expand the characterization to high molecular weight species. This expanded knowledge of the composition of autohydrolysate liquor opens up the potential to develop lucrative co-products from this stream in a commercial biorefinery.

18/00389 Chemical pre-treatment of fugate from biogas stations

Ditl, P. *et al. Biomass and Bioenergy*, 2017, 96, 180–182.

Dealing with the digestate liquid phase from biogas stations has become a problem, due to the rapidly increasing number of biogas stations, tighter legislation, and the nature of the digestate that remains after anaerobic digestion of a biodegradable feedstock. The present solution is a farmland disposal. Standard biological treatment is not applicable because of the extremely high chemical oxygen demand. The method proposed here places chemical pre-treatment of the digestate before the biological stage. This reduces the COD to an acceptable level, from about 100 $kg\,m^{-3}$ to about (2–4) $kg\,m^{-3}$. The separated water phase can then be treated in a standard biological aerobic wastewater treatment plant. The chemical sludge can be treated by composting, together with the biological sludge. With the use of proper additives, a digestate material can be produced that raises the fertilizing and adsorption properties of the soil.

18/00390 Critical factors in energy generation from microalgae

Naraharisetti, P. K. *et al. Energy*, 2017, 120, 138–152.

Fuels from microalgae are being considered as important alternatives to fossil fuels. This work identifies the challenges and opportunities for research in the production of energy from microalgae. The most important challenge facing this alternative resource is the energy generation efficiency (EGE) when microalgae are used for the generation of energy. EGE is about 35% for coal fired power plants while integrated gasification fuel cell cycle (IGFC) and advanced-IGFC (A-IGFC) have an efficiency of over 50%. Other challenges include, achieving a high titre of 2 g/l, a high lipid content of up to 30% and a high CO_2 mass transfer efficiency. It was observed that the process of energy generation from microalgae has good positive energy balance if the EGE can be improved to greater than 50% by developing IGFC/A-IGFC technologies. Other challenges come from energy spent in dewatering, loss of energy when solvents are recycled during the process of lipid extraction, use of energy in the form of methanol and energy used in recycling excess methanol if biodiesel is produced, and energy used in the production of nutrients, among others. Hence, future research must be targeted at minimizing the energy input in these processes.

18/00391 Demand-driven biogas production in anaerobic filters

Lemmer, A. and Krümpel, J. *Applied Energy*, 2017, 185, 885–894.

The growth in electricity generated from renewable energy sources is posing challenges for grid stability and the need to counter balance the intermittent power supply by these sources. Biogas technology can offer such grid services by adapting biogas production to balance the demand and subsequent electricity production of the combined heat and power unit. Innovative plant designs, such as two-staged anaerobic digestion, could possibly adapt to imbalances in the electricity grid within shorter time frames than traditional continuously stirred tank reactors (CSTR). The scope of this research paper was to demonstrate the feasibility of operating an anaerobic filter for highly flexible gas production. The repeatability of this type of operation was examined to demonstrate its predictability. Based on gas production profiles, a measure of responsiveness was introduced to determine whether and how rapidly adaptations to the production process are possible. Furthermore, the influence of substrate composition was tested and finally a carbon balance was derived to evaluate operation performance. The results indicated that anaerobic filters are well suited for flexible gas production and the results were well reproduced under the conditions presented. Substrate composition was found to have no effect on increasing the rate of methane production. The pH value in the reactor did have an effect on the solubility of CO_2 and HCO_3^- and therefore marked an important parameter that determines biogas composition, especially under varying organic loading rates. The carbon balance had showed that the largest output fraction is CH_4, followed by CO_2, inorganic carbon, dissolved organic carbon and particulate carbon with varying shares depending on the experimental phase.

18/00392 Design of biofuel supply chains with variable regional depot and biorefinery locations

Ng, R. T. L. and Maravelias, C. T. *Renewable Energy*, 2017, 100, 90–102.

This study proposes a multi-period mixed-integer linear programming (MILP) model for the design and operational planning of cellulosic biofuel supply chains. Specifically, the proposed MILP model accounts for biomass selection and allocation, technology selection and capacity planning at regional depots and biorefineries. Importantly, it considers the location of regional depots and biorefineries as continuous optimization decisions. Approximation and reformulation methods are introduced for the calculation of the shipments and transportation distance in order to obtain a linear model. The authors illustrate the applicability of the proposed methods using two medium-scale examples with realistic data.

18/00393 Effects of waste fish oil biodiesel on diesel engine combustion characteristics and emission

Gharehghani, A. *et al. Renewable Energy*, 2017, 101, 930–936.

In this study, the combustion characteristics, performance and exhaust emissions of conventional diesel fuel and biodiesel produced from waste fish oil (WFO) and its blends (B25, B50, B75) were compared experimentally. A single-cylinder E6 Ricardo engine was used to perform the tests under steady state conditions and engine load range. In-cylinder pressure, exhaust emissions, fuel consumption and also intake and exhaust gas temperatures were recorded during experiments to analyse the gathered data. Results revealed that waste fish oil biodiesel leads to higher in-cylinder pressure together with shorter heat release rate duration when compared to common diesel fuel. Also, more stable combustion without large cycle-to-cycle variations could be reached by using biodiesel and its blends. Analyses showed that biodiesel has about 2.92% more gross thermal efficiency and about 1.1% lower combustion loss when compared with the diesel fuel, averagely throughout all engine loads. CO emission concentration for biodiesel and its blends is reduced with a gentle slope (5.2–27%), while significant reduction occurred for UHC (11.6–70%). Oxygen content of biodiesel led to more efficient combustion and as result about 7.2% increase in CO_2 averagely while NO_x emission is increased also (1.9–12.8%) by using the biodiesel and its blends.

18/00394 Enhanced biodiesel production from *Jatropha* oil using calcined waste animal bones as catalyst

Nisar, J. *et al. Renewable Energy*, 2017, 101, 111–119.

This study is focused on the investigation of animal bones modified with potassium hydroxide (KOH) as heterogeneous solid base catalyst for transesterification of non-edible *Jatropha* oil. The prepared catalyst was characterized by energy dispersive X-ray (EDX) spectroscopy, powder X-ray diffraction (XRD), scanning electron microscopy (SEM) and thermo-gravimetric analysis (TGA). The prepared catalyst had a high catalytic activity for transesterification. In addition, the catalyst had excellent stability, there by having potential use as a heterogeneous catalyst for biodiesel production from *Jatropha* oil with a high free fatty acid (FFA) yield. The experimental results revealed the optimal parametric conditions, viz. methanol/oil molar ratio, 9 : 1, calcination temperature, 900 °C and catalyst concentration, 6.0 wt % of oil corresponding to a maximum fatty acid methyl esters (FAME) yield of 96.1% at temperature of 70 ± 3 °C in reaction time of 3 h. Reusability results of the prepared catalyst confirmed that it could be reutilized up to four times without losing much activity, thus giving birth to a potentially applicable possibility in biodiesel production.

18/00395 Evaluation of apricot (*Prunus armeniaca* L.) seed kernel as a potential feedstock for the production of liquid bio-fuels and activated carbons

Fadhil, A. B. *Energy Conversion and Management*, 2017, 133, 307–317.

Production of liquid bio-fuels (biodiesel and bio-oil) as well as activated carbon from one non-edible feedstock, apricot (*Prunus armeniaca* L.) seed kernel was the main objective of the present research work. The oil was extracted from apricot seed kernel with a yield of 49.44% w/w of kernels. Potassium hydroxide-catalysed transesterification of apricot (*P. armeniaca* L.) seed kernel oil with methanol and ethanol was then applied to produce methylic and ethylic, respectively. Properties of the obtained biodiesels were evaluated and found conformed to ASTM D 6751 limits. The apricot de-oiled seed kernel was pyrolysed in a semi-batch reactor for bio-oil production. The effect of the pyrolysis temperatures (350, 400, 450, 500, 550 and 600 °C), pyrolysis time (30, 60, 90, 120 and 150 min) and feed particles size (0.25, 0.40, 0.59 and 0.84 mm) on the bio-oil yield was investigated. The maximum production of bio-oil (43.66% w/w) was achieved at a pyrolysis temperature of 450 °C, 60 min pyrolysis time and a feed particles size of 0.25 mm. The bio-oil obtained under the optimal conditions was characterized by the elemental analysis, FTIR spectroscopy and column chromatography. The FTIR analysis of the produced bio-fuel indicated that it composes mainly of alkanes, alkenes, ketones, carboxylic acids and amines. Properties of the resulting bio-oil were analysed in terms of calorific value, density, flash point, pH, acid value, pour point and refractive index. The properties were close to those of petroleum fractions and comparable to those of other bio-oils published in literature. Referring to the experimental results, the obtained bio-oil can be utilized as an important source of alternative fuel and chemicals. The chemical activation method by using sodium hydroxide as the activating agent was utilized to convert the bio-char into activated carbon. The effect of the process parameters including the activation temperatures (400, 500, 600, 700 and 800 °C), activation time (30, 60, 90, 120 and 150 min) and feed particles size (20, 30, 40 and 60 mesh size) on the yield, iodine adsorption number and surface area of the obtained activated carbons were investigated. The optimal activated carbon sample was obtained at 600 °C activation temperature, 90 min activation time and a feed size of 60 mesh. The resulting activated carbon showed good characteristics to be used as adsorbent in water purification as indicated by scanning electron microscope and FTIR spectroscopy.

18/00396 GIS-based allocation of herbaceous biomass in biorefineries and depots

Gonzales, D. S. and Searcy, S. W. *Biomass and Bioenergy*, 2017, 97, 1–10.

While sufficient biomass has been identified to meet the renewable fuel standard (RFS2) targets by previous studies, availability does not equal access. The objective here was to quantify the potential accessible and stranded herbaceous biomass from different scenarios of predicted available biomass in both Texas and the USA. The location and size of potential biorefineries and depots was determined using the geographic location of suitable lands for biomass, the transportation infrastructure and published economic constraints for minimum biomass supplied to a facility within a specified neighbourhood. The GIS-based heuristic addresses the capacitated facility location problem by distributing potential biomass along a county's suitable lands. Road and rail proximity optionally was included in the algorithm. The total stranded biomass in Texas was 28% of the total available biomass. Including the constraint of the transportation network accessibility (rail and appropriate roads) when determining facility location increased the total stranded biomass to 33%. Using county centroids as supply points and potential facilities led to an increase of 7% in total biomass captured by all facilities in Texas when compared to the raster-based heuristic. The nationwide accessible biomass is 90% of the available biomass, 78% of which is captured by biorefineries. In total, 77 biorefineries and 171 depots were identified in the USA, which projects to 184 million Mg $year^{-1}$ delivered to biorefineries and depots, or 65.3 billion litres of advanced biofuels, more than the targeted 60 billion litres of advanced cellulosic biofuel in the RFS2.

18/00397 Harnessing the synergies between lipid-based crystallization modifiers and a polymer pour point depressant to improve pour point of biodiesel

Mohanan, A. *et al. Energy*, 2017, 120, 895–906.

A series of binary mixture additives made of a pour point depressant (PPD) and a vegetable oil based crystallization modifier (VOCM) have been used to substantially improve the cold flow performance of fatty acid methyl esters (FAME) of soybean oil (Soy1500). An apparatus improving on the ASTM methods was designed to measure the cloud point (CP) and pour point (PP). The mixtures dramatically altered Soy1500 crystallization from nucleation to aggregation, and delivered PP depressions reaching 30 °C. The effect was confirmed to be due to synergistic effects wherein the VOCM delays the nucleation by first combining with the saturated FAME of the biodiesel then growing structure specific crystal surfaces that effectively adsorb the PPD which provides barriers to agglomeration. The VOCM-PPD mixture constrains the biodiesel microstructure to very small crystals that are prevented from aggregating over an extended temperature range, leading to a significant depression in the PP. The most dramatic effects were achieved when the PPD is combined in optimal concentration with a VOCM having a structural element which initiates packing and another that prevents further crystallization. Importantly, the results and understanding gathered from the study can be used for the design of highly functional cold flow improver cocktail additives.

18/00398 In-depth study of continuous production of biodiesel using supercritical 1-butanol

Farobie, O. *et al. Energy Conversion and Management*, 2017, 132, 410–417.

The continuous production of biodiesel from canola oil in supercritical 1-butanol (SCB) was thoroughly examined in order to investigate the detailed reaction behaviour and elucidate the reaction kinetics. A continuous reactor was employed, and experiments were carried out at reaction temperatures of 270–400 °C, residence times of 5–30 min, a pressure of 20 MPa, and an oil-to-1-butanol molar ratio of 1 : 40. The factors affecting the product yield, such as temperature and time, were investigated and discussed in detail. The result showed that the highest biodiesel yield of 94.73 mol% was achieved at 400 °C within 14 min. The detailed kinetic model describing the transesterification of canola oil in SCB agreed well with the experimental data. The corresponding reaction rate constants and activation energies were determined. In comparison to supercritical methanol, supercritical ethanol, and supercritical 1-propanol, the reactivity of SCB was the lowest.

18/00399 Influence of mechanical pretreatment and organic concentration of Irish brown seaweed for methane production

Montingelli, M. E. *et al. Energy*, 2017, 118, 1079–1089.

The European Commission opened a discussion about limiting first generation food-based biofuels in favour of advanced biofuels. The main reason was to limit the uncertainty in estimates of indirect land use change emissions (ILUC) of food based biofuels. Brown seaweeds

represent a valuable solution. The lack of lignin makes them suitable for degradation processes such as anaerobic digestion (AD). The main output of AD is biogas which can be upgraded to biomethane and used as a transport fuel. The most common Irish brown seaweeds namely *Laminaria* sp. And *Ascophyllum nodosum* were subject to AD. The effects of beating pre-treatment time (5–10–15 min) and changes in the seaweeds volatile solids (VS) concentration (1–2.5–4%) on methane production were investigated through a response surface methodology (RSM). *Laminaria* sp. showed the highest methane yield of 240 ml CH_4 g^{-1} VS when the pre-treatment time was set at 15 min and at VS concentration of 2.5%. In the case of *A. nodosum*, the best yield of 169 mL CH_4 g^{-1} VS was found at the longest pre-treatment time tested and at the minimum concentration of VS. The RSM analysis revealed that the VS concentration had the strongest impact on the methane yield.

18/00400 Influence of zero valent iron nanoparticles and magnetic iron oxide nanoparticles on biogas and methane production from anaerobic digestion of manure

Abdelsalam, E. *et al. Energy*, 2017, 120, 842–853.

In this study, nanoparticles (NPs) were hypothesized to enhance the anaerobic process and to accelerate the slurry digestion, which increases the biogas and methane production. The effects of NPs on biogas and methane production were investigated using a specially designed batch anaerobic system. For this purpose, a series of 2 L biodigesters were manufactured and implemented to study the effects of the nanoparticles of iron (Fe) and iron oxide (Fe_3O_4) with different concentrations on biogas and methane production. The best results of NPs additives were selected based on the statistical analysis (least significant difference using M-Stat) of biogas and methane production, which were 20 mg/L Fe NPs and 20 mg/L Fe_3O_4 magnetic NPs ($p < 0.05$). The aforementioned NPs additives delivered the highest biogas and methane yields in comparison with their other concentrations (5, 10 and 20 mg/L), their salt ($FeCl_3$) and the control. Furthermore, the addition of 20 mg/L Fe NPs and 20 mg/L Fe_3O_4 magnetic NPs significantly increased the biogas volume ($p < 0.05$) by 1.45 and 1.66 times the biogas volume produced by the control, respectively. Moreover, the aforementioned additives significantly increased the methane volume ($p < 0.05$) by 1.59 and 1.96 times the methane volume produced by the control, respectively. The highest specific biogas and methane production were attained with 20 mg/L Fe_3O_4 magnetic NPs, and were 584 ml Biogas g^{-1} VS and 351.8 ml CH_4 g^{-1} VS, respectively compared with the control which yielded only 352.6 ml Biogas g^{-1} VS and 179.6 ml CH_4 g^{-1} VS.

18/00401 Optimal location of biorefineries considering sustainable integration with the environment

López-Díaz, D. C. *et al. Renewable Energy*, 2017, 100, 65–77.

A typical biorefining supply chain exerts substantial impact on the regional water resources. Indeed, a complex relationship exists between the production of biomass, the processing of biomass into fuels and chemicals, the usage of fresh water, and the discharge of wastewater. This paper introduces an optimization framework for the design of a biorefining system while accounting for the interactions with the surrounding watershed. Special attention is paid in the use of fresh water and the discharge of wastewater to the surrounded watershed. The optimization approach also accounts for the selection of feedstocks, location of cultivation sites and biomass processing facilities, and conversion technologies. Economic and environmental objectives are used. A case study for the central-west part of Mexico is presented. The results show that economic gains may be achieved while optimizing water usage and discharge and satisfying watershed constraints.

18/00402 Optimization of hydrothermal pretreatment for co-utilization C-5 and C-6 sugars of cassava alcohol residue

Lu, H. *et al. Energy Conversion and Management*, 2017, 132, 251–260.

Hydrothermal reaction was first applied to pre-treat cassava alcohol residue for realizing the co-utilization of xylose and glucose to assume fermentation ethanol. This work focused on the influence of hydrothermal pre-treatment conditions on ethanol production. Hydrothermal reaction was used to explore the maximum xylose and glucose yields, in respect to reaction temperature (120–240 °C), solid–liquid ratio (0.023–0.150) and reaction time (15–120 min). The results showed that the suitable conditions were at 180–200 °C, for 45–60 min and with 10–12.5% solids. In this range, the conjunct of xylose and glucose would reach the maximum, which can make full use of hemicellulose and cellulose in cassava alcohol residue. According to the results, respond surface methodology (RSM) based on Box–Behnken design was used to further optimize the three independent variables for the highest ethanol by co-utilization of xylose and glucose. RSM revealed that the effect of temperature on ethanol production was much more significant than the effect of reaction time and solid-liquid ratio, and the highest ethanol production was 70.6 mg/g that was close to the experiment value of 69.5 mg/g at 193 °C for 51 min and with 11.5% solids. Furthermore, the crystallinity and morphology of the untreated and pre-treated cassava alcohol residue were investigated to assess the effect of hydrothermal pre-treatment by scanning electron microscopy and X-ray diffraction, respectively.

18/00403 Optimized location of biomass bales stack for efficient logistics

Subhashree, S. N. *et al. Biomass and Bioenergy*, 2017, 96, 130–141.

Producers often aggregate bales into stacks before transporting these bales to an outlet for consumption or delivery to industrial applications. Efficiency improvement in this infield bale logistics will be beneficial. To address this an R simulation program involving five methods for field stack location, namely field middle, middle data range, centroid, geometric median, and medoid, as well as origin (a direct aggregation method to outlet), were developed. These methods were evaluated against field areas, ranging from 0.5 to 520 ha, for infield bale logistics (aggregation, transport, and total) using Euclidean distances. The simulation used several input field variables, laid out bales based on yield variation, determined optimized bale stack locations of methods, and evaluated distances of aggregation to the stack, transport from the stack to the outlet, and total logistics. The origin method used 1-bale handling tractor for direct aggregation to the outlet, while others formed the bale stacks and transported bales to the outlet using six-bales/trip equipment. Results indicated for aggregation that geometric median was the best, followed by field middle or centroid, middle data range, medoid, and finally origin. Methods aggregation were about 76% and transport about 24% of the total (for > 2 ha); and total distance were about 65% of the origin. ANOVA, excluding origin, indicated that all methods were not significantly different ($p < 0.05$) for the areas studied. The 'field middle' was recommended as an easy and practical method for locating field stacks. Fitted power models described well ($R^2 > 0.99$) all the logistics distances.

18/00404 Permittivity of diesel fossil fuel and blends with biodiesel in the full range from 0% to 100%: application to biodiesel content estimation

Corach, J. *et al. Fuel*, 2017, 188, 367–373.

The relative permittivity of diesel fossil fuel and blends with biodiesel from soybean, in the full range from pure diesel to 100% biodiesel, was determined at temperatures between 298.0 and 333.0 K (controlled within ±0.1 K), using an airtight cell. Measurements were made in the frequency range from 1 to 100 kHz; this frequency range is suitable for the use of low-cost, portable equipment and also for the development of automotive sensors. The relative uncertainty of the measurements was below 1%. Experimental values of permittivity were satisfactorily fitted to a simple model as a function of temperature and composition. The RMS uncertainty of the fitting was 1.2%. The model parameters were determined from experimental results and verified by multiple regression analysis, with very good agreement. In addition, a model was proposed to estimate the composition of diesel/biodiesel blends from permittivity and temperature measurements. The parameters of the model were obtained by a multiple regression analysis; the RMS uncertainty of the composition estimation was below 2.5%. The results presented in this work describe accurately the dependence of the permittivity of diesel fuel with temperature and also validate and extend previously reported models for biodiesel-rich blends with diesel fossil fuel, allowing the estimation in the full composition range with good accuracy.

18/00405 Protonated and layered transition metal oxides as solid acids for dehydration of biomass-based fructose into 5-hydroxymethylfurfural

Zhong, J. *et al. Journal of Energy Chemistry*, 2017, 26, (1), 147–154.

A serial of protonated and layered transition metal oxides, including layered $HTaWO_6$, $HNbMoO_6$ as well as $HNbWO_6$, were synthesized by solid-state reaction and ion-exchange. The layered $HTaWO_6$ has been systematically studied as a solid acid to realize the dehydration of fructose to 5-hydroxymethylfurfural (HMF). The transition metal oxide samples were characterized with ICP-OES, EDS, XRD, XPS, SEM, TGA, FT-IR, N_2 adsorption–desorption and NH_3-TPD. The influential factors such as reaction temperature, reaction time, solvent, catalyst amount and substrate concentration were deeply investigated. The optimized fructose conversion rate of 99% with HMF yield of 67% were achieved after 30 min at 140 °C in dimethylsulfoxide.

18/00406 Resiliency optimization of biomass to biofuel supply chain incorporating regional biomass pre-processing depots

Maheshwari, P. *et al. Biomass and Bioenergy*, 2017, 97, 116–131.

Biomass to biofuel supply chain is subject to several potential disruptions such as flood, drought, pest attack, and equipment failure. These disruptions must be considered while designing the supply chain; especially if capital cost intensive components such as regional biomass pre-processing depots (RBPD) are to be implemented. This work develops a supply chain design optimization model that incorporates

the possibility of such disruptions at the design stage. The objective function is the sum of the total cost incurred during the non-disruption and disruption scenarios weighted by their respective probability of occurrence. This also quantifies the expected disruption cost (EDC) on the operation of the supply chain. The decision variables are the locations and capacities of RBPDs and biorefinery, as well as the biomass flow across the supply chain. The model was applied to two separate case studies, namely, procurement of corn stover from farms arranged in a generic grid pattern, and procurement of corn stover, switchgrass, and Miscanthus for a region of 13 counties in Southern Illinois. The simulation results showed that the consideration of resiliency in design reduced the EDC of supply chain by up to 38% by optimizing the RBPD locations. The results were shown to depend on the intensity and nature of disruptions. This was especially true for feedstock with higher yield such as Miscanthus. Local parameters such as yield and biomass price also affected the optimal results. Moreover, the presence of RBPDs was shown to increase supply chain resiliency.

18/00407 Subcritical and supercritical water gasification of humic acid as a model compound of humic substances in sewage sludge

Gong, M. *et al. The Journal of Supercritical Fluids*, 2017, 119, 130–138.
Humic acid is a model compound of sewage sludge that occurs as a result of decomposing organic matter in wastewater. In this study, humic acid gasification was performed at variable subcritical and supercritical water temperatures (325–600 °C), feed concentration (10–25 wt%) and reaction time (30–90 min). High H_2 yield of 0.79 mol/kg was obtained at 600 °C, 15 wt% humic acid and 75 min without any catalyst. Catalysts such as K_2CO_3, $Ni/Al_2O_3–SiO_2$, $FeCl_3$ and $ZnCl_2$ were examined to enhance H_2 production and humic acid degradation. While H_2 yield increased exponentially with rising $FeCl_3$ loading, $Ni/Al_2O_3–SiO_2$ and K_2CO_3 reduced H_2 yield due to bimolecular condensation and catalyst deactivation. Maximum yield of H_2 (4.09 mol/kg) and total gases (6.20 mol/kg) were obtained with 15 wt% humic acid and 15 wt% $FeCl_3$ at 600 °C and 75 min. Elevated temperatures and high $FeCl_3$ loading promoted the degradation of humic acid with higher gas yields and fragmented surface morphology in char residues.

18/00408 Third generation algae biofuels in Italy by 2030: a scenario analysis using Bayesian networks

Gambelli, D. *et al. Energy Policy*, 2017, 103, 165–178.
This study analysed the potential for biofuels from microalgae in the Italian biofuels context. The scenario analysis considers alternative pathways for the adoption of biofuels from microalgae by the year 2030. The scenarios were developed using a probabilistic approach based on Bayesian networks, through a structured process for elicitation of expert knowledge. The authors have identified the most and least favourable scenarios in terms of the expected likelihood for the development of the market of biofuels from microalgae, through which they have focused on the contribution of economic and policy aspects in the development of the sector. A detailed analysis of the contribution of each variable in the context of the scenarios is also provided. These data represent a starting point for the evaluation of different policy options for the future biofuel market in Italy. The best scenario shows a 75% probability that biofuels from microalgae will exceed 20% of the biofuel market by 2030. This is conditional on the improvement and development of the technological changes and environmental policies, and of the markets for bioenergy and novel foods derived from microalgae.

Geothermal energy

18/00409 3D transient heat transfer numerical analysis of multiple energy piles

Cui, Y. and Zhu, J. *Energy and Buildings*, 2017, 134, 129–142.
This paper presents a three-dimensional (3D) transient heat transfer numerical model for multiple energy piles based on the finite volume method (FVM). The initial and boundary conditions are established and the effects of 'thermal short-circulating' between two pipes of a U-tube in energy pile are investigated. Thermal partial differential equations are discretized at the spatial nodal points and solved by linear approximation method. Temperature variations of working fluid, energy pile and its surrounding soil from simulation program are compared with experimental data to validate the developed model. In addition, the influences of fluid flow rate and U-tube shank spacing are analysed. It is established that the shank spacing should be set in a range of 0.06–0.10 m to reduce heat transfer between the two pipes and meet the structural requirement. Meanwhile, the flow rate should be controlled in a range of 0.5–0.7 m^3/h to avoid the low outlet fluid temperature and decrease the influence of 'thermal short-circuiting'.

18/00410 An appropriate use of the thermal response test for the design of energy foundation piles with U-tube circuits

Zarrella, A. *et al. Energy and Buildings*, 2017, 134, 259–270.
Energy foundation piles can be an efficient cost-effective solution for ground source heat pump applications. As they are very different from standard ground heat exchangers, numerical or analytical models usually used to investigate their thermal performance must be carefully analysed before they can be applied. The total length of ground heat exchangers is a critically important factor in the overall design of a ground source heat pump. Ground thermal properties are the primary parameters affecting the size of ground heat exchangers. The thermal response test is the most commonly used procedure to determine the ground's thermal conductivity. The current study investigated a thermal response test on a 20 m long energy foundation pile equipped with a double U-tube circuit. The test measurements were interpreted using both the infinite line source model and inverse numerical analysis by means of a detailed model that was able to consider both the actual geometry of the pile and the axial heat transfer. The results indicated an approximately 50% difference between the two values of ground thermal conductivity. The effect of this evaluation on the calculation of the energy piles' total length was first investigated utilizing a method outlined in the literature. The consequences on the long term energy performance of a ground source heat pump system were then investigated using numerical simulations and taking into consideration the effect of the spacing between the foundation piles. It was found that the total length calculated using the result based on the infinite line source model was about 20% lower than that obtained using the inverse numerical approach. An approximately 10% difference in the heat pump's seasonal energy efficiency was also found.

18/00411 Evaluation of the impact of the thermal shunt effect on the U-pipe ground borehole heat exchanger performance

Sandler, S. *et al. Geothermics*, 2017, 65, 244–254.
A U-pipe ground borehole heat exchanger (BHE) is the most commonly used device for heat extraction from the ground. The amount of extracted heat depends on two interacting heat transfer processes – between the ground and the carrier fluid, and between the pipes. Heat flow between the U-pipe legs is called the thermal shunt effect (TSE). In this paper, a steady-state numerical model has been used to assess the contribution of TSE to the overall U-pipe performance. As the model requires borehole wall temperature as input, a CFD analysis has been performed to determine how this temperature is influenced by elimination of TSE. The analysis has shown that reducing pipe-to-pipe heat flow has no substantial impact on the borehole wall temperature. Fluid temperature profiles have been calculated for all possible pipe arrangements in a heat exchanger with the borehole diameter of 152 mm, pipe diameters in the range of 30.4–45.6 mm and borehole depths ranging from 30 to 200 m. Results indicate that thermal shunting becomes aggravated by decreasing pipe-to-pipe distance or increasing pipe diameters and borehole depths. The maximum loss of 35% in the U-pipe thermal performance has been observed in the range of investigated parameters, which proves the necessity of TSE elimination.

18/00412 Feasibility of geothermal heat exchanger pile-based bridge deck snow melting system: a simulation based analysis

Han, C. and Yu, X. (B.) *Renewable Energy*, 2017, 101, 214–224.
A snow melting system based on geothermal heat exchanger pile is an innovative technology that combines geothermal energy with structural foundation. It overcomes the problems of conventional chemical based snow melting in mitigating infrastructure corrosion and negative environmental effects. By integrating the underground heat exchanger into pile foundation that support the bridge structure, it effectively reduces the installation cost of geothermal system. This paper analyses the applicability and performance of such snow melting system for different regions. Energy demand for snow removal is firstly determined with ASHRAE criteria. A holistic 3D simulation model is developed to predict the energy extraction rate under different operation conditions. A hypothetical bridge deck [200 m length by 14.8 m (four lanes) width] is analysed to assess the feasibility of geothermal heat exchanger pile based snow melting system for 10 cities representing a variety of climatic regions of the USA. The number of pile foundation required for snow melting is used as indication of the technical feasibility. The results show that its feasibility and performance in bridge deck snow removal is dependent upon the geological and snow conditions of a particular region, as well as the design snow removal criteria.

18/00413 Fluid injection in enhanced geothermal systems: a study on the detectability of self-potential effects and on their correlation with induced seismicity

Troiano, A. *et al. Geothermics*, 2017, 65, 280–294.

This study presents a numerical modelling aimed at investigating nature and role of the self-potential (SP) anomalies induced by water injection in boreholes at the Soultz-sous-Forêts (SsF) hot dry rock enhanced geothermal field. The overpressure due to the fluid stimulation is considered as source of the streaming potential effects in rocks, responsible on their turn of the SP anomalies observed at the ground surface. The numerical simulations have been realized by a combined application of the TOUGH2 and Comsol Multiphysics codes, which had already been successfully used to predict Coulomb stress changes in rocks induced by a fluid injection cycle. Two synthetic cases are investigated. At first, a simulated injection cycle in a single borehole has been modelled, consisting in the reconstruction of the overpressure and SP temporal and spatial evolutions induced by the hydraulic stimulation of the rock. The main result is that the front of the SP anomaly follows the overpressure front, with the time delay between the two fronts decreasing at increasing distance from the well. The second case takes into consideration a real injection experiment performed in 2003 at SsF, which has allowed to examine the induced seismicity. The simulated SP response to this real injection cycle shows that the SP temporal evolution is essentially a post-seismic effect. The conclusion from the simulations is that SP measurements can be used to localize the main features of the fluid flow into the reservoir.

18/00414 Geochemical study of the Sakalol-Harralol geothermal field (Republic of Djibouti): evidences of a low enthalpy aquifer between Manda-Inakir and Asal rift settings

Awaleh, M. O. *et al. Journal of Volcanology and Geothermal Research*, 2017, 331, 26–52.

Eighty-six sodium bicarbonate to sodium chloride hot springs and four water wells in the Tadjourah Region of Djibouti were investigated for major, minor (B, Br, F, Sr, Li) chemistry and isotope composition of water and dissolved components ($^{87}Sr/^{86}Sr$, $^{11}B/^{10}B$, $^{13}C/^{12}C$ and ^{14}C of DIC, $^{34}S/^{32}S$ and $^{18}O/^{16}O$ of sulfate). The deep saline Na–Cl reservoir at 143 °C shows affinity with the shallow geothermal water from the 'active' Asal rift. Asal water is a diluted and recycled seawater component with the major cation composition obliterated by equilibration with Stratoid basalt. Locally, the deep reservoir is differentiated in term of recharge, and re-equilibration with rocks and mixing. In particular, two spring groups reveal contributions from evaporites typical of the 'passive' graben setting of the Afar. A model on $^{34}S/^{32}S$ and $^{18}O/^{16}O$ demonstrates the isotope imprint of magmatic SO_2 disproportionation on dissolved and solid sulfate, whose values probably persists in a sedimentary environment without trace of seawater. On the other hand a seawater signature, modified by mixing and secondary fractionation effects, is partially maintained according to the boron isotope composition (up to + 27.4‰). Temperature estimation in low-enthalpy geothermal reservoirs is notoriously difficult, especially where mixing with fluids of differing genesis and/or conduction cooling take place. From a geothermometric point of view, the multi-method approach followed in this study (up-to-date theoretical and thermodynamic equations, ad-hoc silica geothermometers inferred from local rocks, checking of the results on a $^{18}O\alpha_{sulfate\text{-}water}$ vs temperature diagram) provides some insights and perspectives on how to tackle the problem.

18/00415 Geophysical image of the hydrothermal system of Merapi volcano

Byrdina, S. *et al. Journal of Volcanology and Geothermal Research*, 2017, 329, 30–40.

This study presents an image of the hydrothermal system of Merapi volcano based on results from electrical resistivity tomography (ERT), self-potential, and CO_2 flux mappings. The ERT models identify two distinct low-resistivity bodies interpreted as two parts of a probably interconnected hydrothermal system: at the base of the south flank and in the summit area. In the summit area, a sharp resistivity contrast at ancient crater rim Pasar-Bubar separates a conductive hydrothermal system (20–50 Ω m) from the resistive andesite lava flows and pyroclastic deposits (2000–50,000 Ω m). The existence of preferential fluid circulation along this ancient crater rim is also evidenced by self-potential data. The significative diffuse CO_2 degassing (with a median value of 400 g m^{-2} d^{-1}) is observed in a narrow vicinity of the active crater rim and close to the ancient rim of Pasar-Bubar. The total CO_2 degassing across the accessible summital area with a surface of 1.4×10^5 m^2 is around 20 t d^{-1}. Before the 2010 eruption, it was estimated that a higher value of the total diffuse degassing from the summit area (about 200–230 t d^{-1}). This drop in the diffuse degassing from the summit area can be related to the decrease in the magmatic activity, to the change of the summit morphology, or, more likely, to a combination of these factors. On the south flank of Merapi, the resistivity model shows spectacular stratification. While surficial recent andesite lava flows are characterized by resistivity exceeding 100,000 Ω m, resistivity as low as 10 Ω m has been encountered at a depth of 200 m at the base of the south flank and was interpreted as a presence of the hydrothermal system. No evidence of the hydrothermal system is found on the basis of the north flank at the same depth. This asymmetry might be caused by the asymmetry of the heat supply source of Merapi whose activity is moving south or/and to the asymmetry in topography caused by the presence of Merbabu volcano in the north. On the basis of these results, the authors suggest that stratified pyroclastic deposits on the south flank of Merapi screen and separate the flow of hydrothermal fluids with the gaseous part rising through the crater rims, while the liquid part is flowing downwards to the base of the edifice.

18/00416 Lifetime design strategy for binary geothermal plants considering degradation of geothermal resource productivity

Budisulistyo, D. *et al. Energy Conversion and Management*, 2017, 132, 1–13.

This work proposes a lifetime design strategy for binary geothermal plants which takes into account heat resource degradation. A model of the resource temperature and mass flow rate decline over a 30-year plant life is developed from a survey of data. The standard approach to optimize a basic subcritical cycle of *n*-pentane working fluid and select component sizes is used for the resource characteristics in years 1, 7, 15 and 30. The performances of the four plants designed for the different resource conditions are then simulated over the plant life to obtain the best lifetime design. The net present value and energy return on investment are selected as the measures of merit. The production history of a real geothermal well in the Taupo Volcanic Zone, New Zealand, is used as a case study for the lifetime design strategy. The results indicate that the operational parameters (such as mass flow rate of *n*-pentane, inlet turbine pressure and air mass flow rate) and plant performance (net power output) decrease over the whole plant life. The best lifetime plant design was at year 7 with partly degraded conditions. This condition has the highest net present value at US$6,894,615 and energy return on investment at 4.15. Detailed thermo-economic analysis was carried out with the aim of improving the plant performance to overcome the resource degradation in two ways: operational parameters adjustments and adaptable designs. The results shows that mass flow rates of *n*-pentane and air cooling should be adjusted to maintain the performance over the plant life. The plant design can also be adapted by installing a recuperator and reducing the heat transfer area of preheater and vaporizer.

18/00417 Mechanical behaviour of Australian Strathbogie granite under in-situ stress and temperature conditions: an application to geothermal energy extraction

Kumari, W. G. P. *et al. Geothermics*, 2017, 65, 44–59.

Geothermal heat has now been identified as an effective renewable energy source due to severe environmental impacts created by conventional fossil usage on global climatic change. However, its wide application has been limited due to the lack of knowledge, particularly of the geothermal conditions of reservoir rocks at elevated temperatures and pressures. Such high temperatures and pressures possibly alter the mechanical properties of reservoir rocks due to the associated micro-structural and mineralogical alterations of the rock mass, which are an important attribute for wellbore stability and stimulation of geothermal reservoirs for safe and effective geothermal energy extraction. This study therefore investigates the stress-strain behaviour under *in situ* stress and temperature conditions by conducting a series of high-pressure, high-temperature tri-axial experiments on Australian Strathbogie granite under four different confining pressures (10, 30, 60, 90 MPa) and four different temperatures (100, 200, 300 °C). The effect of temperature on the mechanical behaviour of rock specimens was studied under tri-axial conditions and the corresponding fracture propagation behaviour was observed using an advanced acoustic emission system. The corresponding micro-structure alteration in granite was observed using SEM analysis. According to the findings, increasing temperature leads to an initial increment in reservoir rock strength and shear parameters followed by reduction, and the trend is aligned with the crack formation pattern of the rock mass. This was further confirmed by the SEM analysis, according to which the rock micro-structure is subject to only minor changes at relatively low temperatures and higher temperatures cause micro-cracks to develop along the rock mass grain boundaries. Furthermore, the conventional Mohr-Coulomb criteria failed to model the stress-strain response of rock under geothermal reservoir conditions, and was therefore modified for the corresponding *in situ* conditions.

18/00418 Oxygen isotope systematics in an evolving geothermal system: Coso Hot Springs, California

Etzel, T. M. *et al. Journal of Volcanology and Geothermal Research*, 2017, 329, 54–68.

Oxygen isotope and clay mineralogy studies have been made on whole rock samples and feldspar separates from three wells along the high temperature West Flank of the Coso geothermal system, California. The reservoir rocks have experienced variable $^{18}O/^{16}O$ depletion, with $\delta^{18}O$ values ranging from primary values of +7.5‰ down to −4.6‰. Spatial patterns of clay mineral distributions in the three wells are not

closely correlated with the distributions expected from measured, pre-production temperature profiles, but do correlate with spatial patterns of $^{18}O/^{16}O$ depletion, indicating that the stability of clay minerals in the three wells is a function of fluid-rock interaction in addition to temperature. Detailed $\delta^{18}O$ measurements in the three wells identify a limited number of localized intervals of extensive $^{18}O/^{16}O$ depletion. These intervals document localized zones of higher permeability in the geothermal system that have experienced significant fluid infiltration, water-rock interaction and oxygen isotopic exchange with the geothermal fluids. The local zones of maximum $^{18}O/^{16}O$ depletion in each well correspond closely with current hot water production zones. Most feldspar separates have measured $\delta^{18}O$ values too high to have completely attained oxygen isotope exchange equilibrium with the reservoir fluid at pre-production temperatures. In general, the lower the $\delta^{18}O$ value of the feldspar, the closer the feldspar approaches exchange equilibrium with the geothermal fluid. This correlation suggests that fracture-induced increases in permeability increase both fluid infiltration and the surface area of the host rock exposed to geothermal fluid, promoting fluid-rock interaction and oxygen isotope exchange. The two most $^{18}O/^{16}O$-depleted feldspar samples have $\delta^{18}O$ values too low to be in exchange equilibrium with the pre-production reservoir fluid at pre-production temperatures. These discrepancies suggest that the reservoir fluid in the West Flank of the Coso geothermal system was hotter and/or had a lower $\delta^{18}O$ value (due to fluid-rock interaction at higher permeability) in the past.

18/00419 Performance measures in geothermal power developements [developments]

Varney, J. *et al. Renewable Energy*, 2017, 101, 835–844.

Geothermal resource assessment requires several input parameters at a time when field information is normally very limited. The power plant efficiency is an important parameter as it affects investment cost and profit. However, there is significant debate in the geothermal industry on the appropriate performance measure to implement. This paper attempts to determine the best performance measures for financial decision making during the exploration stage of geothermal power developments. The authors compare and contrast current performance measures commonly used by the geothermal industry. This includes thermal efficiency, geothermal brine effectiveness, utilization efficiency and enthalpy efficiency. It is shown that enthalpy efficiency, categorized by the geothermal reservoir enthalpy, is the best financial performance measure because it is similar to other measures on most criteria, but superior in terms of comparability across different geothermal sites, while satisfying homoscedasticity. Utilization efficiency, on the other hand, was demonstrated to have the least reliability while requiring additional input parameters. The authors recommend using the modified enthalpy efficiency developed in this work for resource assessment of new geothermal fields, benchmarking with existing development and for comparison with conventional fossil-fuel thermal plants. This should also affect the choice of resource assessment methodology.

18/00420 Predicting permeability of low-enthalpy geothermal reservoirs: a case study from the Upper Triassic – Lower Jurassic Gassum Formation, Norwegian–Danish Basin

Weibel, R. *et al. Geothermics*, 2017, 65, 135–157.

This paper aims at improving the predictability of permeability in low enthalpy geothermal reservoirs by investigating the effect of diagenesis on sandstone permeability. Applying the best fitted porosity–permeability trend lines, obtained from conventional core analysis, to log-interpreted porosity, is crucial in estimating reservoir permeability from logs. Petrographical analysis of sandstones from the Gassum Formation reveals lithological and diagenetic controls on plug permeability and porosity. Porosity–permeability trend lines vary with grain size for the shallowly buried sandstones (<2500 m). Deeply buried sandstones (>2500 m) from a steeply sloping porosity–permeability trend line since the pore-throat diminution due to quartz, ankerite and illite precipitation affects the permeability more than porosity, as evident from mercury injection curves. Permeabilities lower than the general trend for each grain-size group are caused by early diagenetic siderite cement, late diagenetic illitic clays and/or detrital clays. Permeabilities of sandstones deposited under humid well-vegetated conditions in marine and paralic environments, such as the Gassum Formation, are primarily dependent on burial history (maximum burial depth) and depositional environment.

18/00421 Pressure transient analysis of geothermal wells: a framework for numerical modelling

McLean, K. and Zarrouk, S. J. *Renewable Energy*, 2017, 101, 737–746.

The need for numerical models for geothermal pressure transient analysis (PTA) is well recognized. Conventional PTA is based on analytical models which usually do not work for geothermal datasets, therefore PTA is under-utilized by the geothermal industry. A framework for numerical modelling is required to promote comparability of results and increase user-friendliness. A framework is developed in this study using the TOUGH2 simulator and automated using PyTOUGH. A full justification of the grid design and model setup is given. A reference model is then created and subjected to a sensitivity analysis. The only parameter to which the model output is sensitive is the layer thickness of the model. The basic framework is equivalent to the analytical infinite uniform porous reservoir model. An equivalent to the analytical linear impermeable boundary model has also been developed. The framework is then demonstrated by investigating the injection of cold water into a hot reservoir, a major issue for geothermal PTA. The tool is further demonstrated in a case study with datasets before and after deflagration of a well, and was found to produce superior results to the equivalent analytical analysis.

18/00422 Tailor-made risk governance for induced seismicity of geothermal energy projects: an application to Switzerland

Trutnevyte, E. and Wiemer, S. *Geothermics*, 2017, 65, 295–312.

Fully open or partly open geothermal systems can induce potentially damaging seismicity. How this seismicity should be addressed depends on the geothermal system, its operational characteristics, the geological context, exposed buildings, existing infrastructure and populations, and social concern. This paper proposes an initial screening tool, called 'geothermal risk of induced seismicity diagnosis' (GRID), for estimating to what extent induced seismicity is of concern for a specific project. A framework for tailor-made risk governance measures is then recommended, including hazard and risk assessment, social site characterization, seismic monitoring, insurance, structural retrofitting, traffic light systems, information and outreach, and public and stakeholder engagement. The proposed framework is currently customized to Switzerland but can be adapted to other regions or geo-energy applications.

Solar energy

18/00423 12.35% efficient graphene quantum dots/silicon heterojunction solar cells using graphene transparent electrode

Diao, S. *et al. Nano Energy*, 2017, 31, 359–366.

Zero-dimensional graphene quantum dots (GQDs) have lately intrigued intensive interest because of their great promise in energy, optoelectronic, and bio-imaging applications. Herein, the authors demonstrated the fabrication of highly efficient GQDs/n-silicon heterojunction solar cells via a simple solution process. Owing to the unique band structure, the GQDs layer could not only serve as hole transport layer to facilitate the separation of photo-generated electron-hole pairs, but also act as electron blocking layer to suppress the carrier recombination at anode. Moreover, graphene was used as the transparent top electrode for the heterojunction solar cells, ensuring the efficient light absorption and carrier collection. By adjusting the sizes of GQDs and the thickness of GQDs layer, a power conversion efficiency (PCE) as high as 12.35% under AM 1.5 G irradiation was achieved, which represented a new efficiency record for this new-type solar cell. The devices also exhibited excellent stability in air due to the high chemical/physical stability of GQDs and graphene. The successful achievement of the high-efficiency GQDs/Si heterojunction solar cells opens up the opportunities for their potential applications in high-performance and low-cost photovoltaics.

18/00424 A facile molecularly engineered copper (II) phthalocyanine as hole transport material for planar perovskite solar cells with enhanced performance and stability

Yang, G. *et al. Nano Energy*, 2017, 31, 322–330.

Perovskite solar cells (PSCs) demonstrate huge potential in photovoltaic conversion, yet their practical applications face one major obstacle: their instability. As to conventional hole transport materials (HTMs) such as spiro-OMeTAD, their future commercialization maybe hampered for the cost and instability. Here, the authors report a new HTM of copper(II) phthalocyanine with octamethyl-substituted function groups ($CuMe_2Pc$). Unlike the normal edge on orientation of pristine copper(II) phthalocyanine (CuPc), it was found that $CuMe_2Pc$ could form face-on molecular alignment when deposited on perovskite via vacuum thermal evaporation, resulting in higher hole mobility, more condense thin film structure and more hydrophobic surface. These properties are more favourable for hole transport and moisture resistance applications in PSCs. PSCs with planar structure were fabricated and tested, utilizing different phthalocyanines and spiro-OMeTAD as HTMs. PSCs with $CuMe_2Pc$ showed 25% higher power conversion efficiency (PCE) compared with those with CuPc. Furthermore, beneficial from the hydrophobic nature of $CuMe_2Pc$, the devices

with $CuMe_2Pc$ as HTM show improved stability and retained over 95% of their initial efficiencies even after storage in the humidity about 50% for 2000 h without encapsulation. This study demonstrates that $CuMe_2Pc$ is a potential HTM for fabricating low-cost and efficient PSCs with long-term stability.

18/00425 A model-based approach for optical performance assessment and optimization of a solar dish

Xiao, G. *et al. Renewable Energy*, 2017, 100, 103–113.

The solar dish is a point-focusing concentrator with a very high concentration ratio ranging from hundreds to thousands. Practical assessment and optimization methods are necessary to assemble solar dishes with satisfying concentration ratios and flux density distributions, which is very important for the overall solar thermal systems to achieve high efficiency. A solar dish usually consists of many mirror facets installed on a supporting structure with a dual-axis tracking system. Small mirror facets are easy to manufacture, but the alignment of many mirror facets is very challenging. A model-based approach for optical performance assessment and optimization of a solar dish was proposed, and flux density measurements were carried out to validate the approach. The simulation and experimental results showed very good consistency and suggested that the concentration ratio and the intercept factor could be increased from ~500 to ~1500 and 0.66 to 0.9, respectively, after assembly optimization.

18/00426 A novel solar PV MPPT scheme utilizing the difference between panel and atmospheric temperature

Husain, M. A. *et al. Renewable Energy Focus*, 2017, 19–20, 11–22.

This paper puts forward a novel technique employing the thermocouple for tracking maximum power point (MPP) in the photovoltaic systems. This is a rapid and accurate method for tracking the MPP by means of the thermocouple installed beneath the PV panel. It is observed that the temperature of the panel is higher than the atmospheric temperature and this difference in temperature is used in the proposed maximum power point tracker (MPPT). The technique performs swift and efficient tracking as compared to conventional methods. The main lead of this method is that it tracks voltage which has a direct relationship with duty cycle of the converter instead of tracking power. This makes the analysis simpler. Also the thermocouple employed (when used on large scale) can act as an additional power source. The algorithm can be easily implemented and produces accurate results. The system can be comprehended using simple circuitry. The behaviour and performance of the proposed MPPT is shown by simulation and experiment. The exploration is accomplished using the Kotak KM-0018 SPV module. The practical experimentation is performed and the results are found to be in conformity with the simulation results with minor deviations.

18/00427 A practical technique for on-line monitoring of a photovoltaic plant connected to a single-phase grid

Yahyaoui, I. and Segatto, M. E. V. *Energy Conversion and Management*, 2017, 132, 198–206.

Improving the reliability and enhancing the performance of photovoltaic (PV) plants are important objectives that increase the competitiveness of the PV systems, especially for grid connected PV plants, for which, every kilowatt-hour is crucial, since only kilowatt-hours that are fed into the grid are remunerated. Therefore, monitoring and automatic faults detection during the PV panels operation are necessary to ensure the optimal use of the energy generated by the PV plant, and to provide a reliable power supply. In this research paper, two current and voltage indicators are used to analyse and to distinguish, in real-time, the faults related to bypassed PV modules, open-circuits strings and partial shading for a PV plant connected to a single-phase grid. Moreover, the presented strategy allows determining the total number of faulty PV modules and/or strings. The efficiencies of these indicators are tested by experiments, using a control and data acquisition system, which proved the effectiveness of the proposed approach.

18/00428 A review of photovoltaic thermal (PV/T) heat utilisation with low temperature desiccant cooling and dehumidification

Guo, J. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 1–14.

One of the major obstacles to improving solar thermal cooling technologies is the high operating temperature requirements of most solar thermal cooling systems. This paper reviews recent advances that could reduce the required heat source temperatures for solar desiccant cooling to the range of 50–60 °C. These approaches include: (i) isothermal dehumidification (e.g. two-stage dehumidification or internal cooled dehumidification) and (ii) pre-cooling of the entry air with ambient heat sinks (e.g. indirect evaporative cooling or geothermal exchange). These techniques can potentially leads to a more thermodynamically efficient solution for utilizing recovered heat from flat plate photovoltaic thermal (PV/T) collectors for desiccant regeneration. Analysis of the literature shows that obtainable outlet fluid temperatures from existing PV/T systems nearly match the low temperature desiccant cooling and dehumidification applications. Design and operation factors for achieving sufficiently high outlet fluid temperature in flat plate PV/T collectors include (i) maintaining low mass flow rate per collector area, (ii) addition of a glazed cover and (iii) hydraulic channel diameter optimization. These factors are reviewed and case studies of complete solar PV/T desiccant cooling are examined.

18/00429 Amorphous hole-transporting layer in slot-die coated perovskite solar cells

Qin, T. *et al. Nano Energy*, 2017, 31, 210–217.

Perovskite solar cells can be produced by a solution process and have achieved power conversion efficiency over 20% as well as improving long-term stability, offering great potential for a low-cost, high-efficiency photovoltaic technology. An increasing effort has been shifted to Lab-to-Fab translation, where device manufacture is accomplished by using a fully scalable printing process. One remarkable bottleneck for upscaling the device is, however, the lack of scalable hole-transport materials (HTMs) that can form the desired morphology during the printing fabrication. In this manuscript, the authors apply a twisted but fully π-conjugated 2,2′,7,7′-tetrakis(N,N-di-*p*-methoxyphenyl)amine-9,9′-bifluorenylidene (Bifluo-OMeTAD) into slot-die coated devices, which exhibits excellent film forming properties and outperforms the well-known Spiro-OMeTAD HTM. The improved film forming properties of Bifluo-OMeTAD are achieved via molecular design, with the chemical structure of Bifluo-OMeTAD effectively suppressing crystallization during printing. A power conversion efficiency of 14.7% is achieved in the fully slot-die coated devices based on Bifluo-OMeTAD, outperforming previous reported values for all-printed perovskite solar cells. Therefore, Bifluo-OMeTAD has attractive potential to replace Spiro-OMeTAD for the large scale roll-to-roll production of fully slot-die coated perovskite solar cells.

18/00430 Characterization of solar fuels obtained from beech wood solar pyrolysis

Zeng, K. *et al. Fuel*, 2017, 188, 285–293.

Solar pyrolysis of biomass is a smart way to upgrade biomass and, thus, store intermittent solar energy as solar fuels (gas, bio-char and bio-oil). Distribution and energy content of gas, char and oil depend on experimental conditions. In order to determine these characteristics, experiments have been performed at temperatures of 600, 900, 1200 and 2000 °C, heating rate of 50 °C/s and argon flow rate of 6 NL/min. The gas product was analysed by micro-GC. The char product was characterized by CHNS, whereas the oil product was subjected to CHNS, Karl–Fischer titration and GC–MS analysis. The LHVs (lower heating values) for gas, char and oil were determined from empirical equations. The gas product yield and LHV significantly increase with temperature, which is mainly due to more H_2 and CO formation by the enhanced secondary tar reactions. The char and oil characteristics highly depend on the temperature. Their high energy contents show that the obtained char and oil can be utilized as valuable solid and liquid fuels. The biomass energy upgrading due to solar processing is discussed. At optimum temperature 900 °C, it ranges from 38% to 53% accounting for the uncertainty of bio-oil water content.

18/00431 Chemical stability of silicon nitride coatings used in the crystallization of photovoltaic silicon ingots. Part I: stability in vacuum

Selzer, A. *et al. Journal of the European Ceramic Society*, 2017, 37, (1), 69–74.

Photovoltaic silicon is currently grown in silica crucibles coated with an oxidized silicon nitride powder, which acts as an interface releasing agent between the silicon and the crucible. A series of experiments was performed to study the reactions between coating components under high vacuum, varying the temperature, the holding time and the oxygen content in the coating. The results are discussed with the help of a simple analytical model taking into account the diffusive transport of reaction species from the inside of the porous coating to its surface and then their evaporation into the vapour phase.

18/00432 Chemical stability of silicon nitride coatings used in the crystallization of photovoltaic silicon ingots. Part II: stability under argon flow

Drevet, B. *et al. Journal of the European Ceramic Society*, 2017, 37, (1), 75–82.

Processing of photovoltaic silicon by solidification is currently carried out under argon flow in silica crucibles coated with an oxidized silicon nitride powder. A series of experiments was performed to study the reactions between coating components under argon flow by varying the temperature, the holding time and the oxygen content in the coating. The results are discussed with the help of a simple analytical model taking into account the diffusive transport of gaseous reaction species

from the inside of the porous coating to the flowing argon. The conclusions drawn are used to discuss different practical aspects of the photovoltaic silicon crystallization process.

18/00433 Comparative analyses on dynamic performances of photovoltaic–thermal solar collectors integrated with phase change materials

Su, D. *et al. Energy Conversion and Management*, 2017, 131, 79–89.

The operating conditions (especially temperature) of photovoltaic–thermal solar collectors have significant influence on dynamic performance of the hybrid photovoltaic–thermal solar collectors. Only a small percentage of incoming solar radiation can be converted into electricity, and the rest is converted into heat. This heat leads to a decrease in efficiency of the photovoltaic module. In order to improve the performance of the hybrid photovoltaic–thermal solar collector, the authors performed comparative analyses on a hybrid photovoltaic–thermal solar collector integrated with phase change material. Electrical and thermal parameters like solar cell temperature, outlet temperature of air, electrical power, thermal power, electrical efficiency, thermal efficiency and overall efficiency are simulated and analysed to evaluate the dynamic performance of the hybrid photovoltaic–thermal collector. It is found that the position of phase change material layer in the photovoltaic–thermal collector has a significant effect on the performance of the photovoltaic–thermal collector. The results indicate that upper phase change material mode in the photovoltaic–thermal collector can significantly improve the thermal and electrical performance of photovoltaic–thermal collector. It is found that overall efficiency of photovoltaic–thermal collector in 'upper phase change material' mode is 10.7% higher than that in 'no phase change material' mode. Further, for a photovoltaic–thermal collector with upper phase change material, it is verified that 3 cm-thick phase change material layer is excellent both in electrical and thermal performance.

18/00434 Effect of surfactants on the morphologies of TiO_2 particles with high-performance scattering layer in dye-sensitized solar cells

Lekphet, W. *et al. Solar Energy*, 2017, 142, 1–12.

A series of TiO_2 powders with various morphologies were synthesized using surfactant-assisted hydrothermal method by hydrolysing the titanium tetra-isopropoxide (TTIP) precursor. Four types of tetraalkylammonium hydroxide (TANH) surfactants such as tetramethylammonium hydroxide (TMAH), tetraethylammonium hydroxide (TEAH), tetrapropylammomium hydroxide (TPAH), and tetrabutylammonium hydroxide (TBAH) were used before hydrothermal crystallization. The results showed that the surfactants with different alkyl chain length of tetraalkylammonium cations (TAN^+) had a great influence on the morphology, particle size, and crystalline phase of TiO_2 particles. Under the same experimental conditions, the surfactants of TMAH, TEAH, TPAH, and TBAH resulting in the star-, flower-, rod-, and scree-shaped TiO_2 particles (TM-, TE-, TP-, and TB-TiO_2), respectively. The particle sizes were decreased in the range from ~3.6 μm to ~220 nm while increasing the alkyl chain length of the surfactants. All the TiO_2 powders showed an anatase phase besides the TiO_2 prepared from TMAH surfactant. The photovoltaic investigations of these TiO_2 samples as the scattering layer in DSSCs indicated that the TB-TiO_2 based cell exhibited the excellent power conversion efficiency of 9.88%, which was also higher than that of a device which fabricated without a scattering layer (8.83%). Among these scattering layers, TB-TiO_2 has the optimum particle size (~220 nm) with the highest surface area leading to the largest dye adsorption value and an excellent efficiency. In order to further increase the dye adsorption of the photoanodes, the scattering layer was prepared by mixing the large (TB-TiO_2) and small sized (*a*-TiO_2) particles as composites with different weight ratios, leading to the highest efficiency of 10.53% at TB-/*a*-TiO_2 (2 : 3).

18/00435 Exergy analysis of a solar-powered vacuum membrane distillation unit using two models

Miladi, R. *et al. Energy*, 2017, 120, 872–883.

A detailed exergy analysis of a solar powered vacuum membrane distillation (VMD) unit was performed using two models: the ideal mixture model and the model using the thermodynamics properties of seawater. The exergy flow rates of process steam, given by the two models differed of about 18%, on average. Despite these differences, the two models agree that during the step of condensation, the most important fraction of exergy was destroyed. Moreover, in this work, two forms of exergy efficiency are calculated. The overall exergy efficiency of the unit with reference to the exergy collected by the solar collector was 3.25% and 2.30% according to Cerci and Sharqawy models, respectively. But, it was 0.182% and 0.128%, when referenced to the exergy of solar radiation, according to Cerci and Sharqawy models, respectively. Besides, the utilitarian exergy efficiency was 9.96%. Since the heat exchanger, the hollow-fibre module and the condenser have a very high exergy performance, then it can be concluded that the enhancement or reduction of exergy losses will be mainly by recovering heat lost in brine discharges and in the rejection of the cooling water. In addition, the influence of the rejection rate on exergy efficiencies was studied.

18/00436 Experimental study of the dust effect on photovoltaic panels' energy yield

Abderrezek, M. and Fathi, M. *Solar Energy*, 2017, 142, 308–320.

In this paper, the effect of dust on electrical and thermal behaviour of photovoltaic (PV) panels is investigated. For this aim, several types of dusts are considered. Which leads to different panel behaviours in the thermal, optical and electrical aspects. Indeed, it has been shown that light transmission varies with dust type. Laboratory tests using various instruments such as microscope, spectrophotometer, *I–V* PV modules analyser and data logger equipped with thermocouples are carried out. The obtained results show that variations on the physical parameters (grain size and type), level of light transmission and the glazing temperature lead to change in performance of PV panels. The experimental observed behaviours were in accordance with the results obtained using the Energy2D computer simulation code of the thermal behaviour applied to the glazing and PV module (glass, EVA, cell, frame and Tedlar).

18/00437 Extended Kalman filtering to estimate temperature and irradiation for maximum power point tracking of a photovoltaic module

Docimo, D. J. *et al. Energy*, 2017, 120, 47–57.

This paper develops an algorithm for estimating photovoltaic (PV) module temperature and effective irradiation level. The power output of a PV system depends directly on both of these states. Estimating the temperature and irradiation allows for improved state-based control methods while eliminating the need of additional sensors. Thermal models and irradiation estimators have been developed in the literature, but none incorporate feedback for estimation. This paper outlines an extended Kalman filter for temperature and irradiation estimation. These estimates are, in turn, used within a novel state-based controller that tracks the maximum power point of the PV system. Simulation results indicate this state-based controller provides up to an 8.5% increase in energy produced per day as compared to an impedance matching controller. A sensitivity analysis is provided to examine the impact state estimate errors have on the ability to find the optimal operating point of the PV system.

18/00438 High efficiency $CH_3NH_3PbI_3$: CdS perovskite solar cells with $CuInS_2$ as the hole transporting layer

Chen, C. *et al. Journal of Power Sources*, 2017, 341, 396–403.

The $CH_3NH_3PbI_3$: CdS composite films are prepared by a newly developed precursor blending solution method, which are further used to fabricate $CH_3NH_3PbI_3$: CdS perovskite solar cells. The experimental results demonstrate that the introduced CdS effectively improves the light absorption property of the ITO/$CuInS_2$/Al_2O_3/$CH_3NH_3PbI_3$: CdS film stack and decreases the charge recombination in the prepared solar cells due to the formation of $CH_3NH_3PbI_3$/CdS bulk heterojunction. Furthermore, the formed CdS/$CuInS_2$ heterojunction also contributes to the enhanced efficiency. As a consequence, the $CH_3NH_3PbI_3$/CdS bulk heterojunction perovskite solar cells exhibit a maximum power conversion efficiency of (16.5 ± 0.2)%, which is 1.35 times the best efficiency of 12.2% of previously reported CdS/$CH_3NH_3PbI_3$ bilayer solar cell. In addition, this efficiency is a 59% improvement compared with the efficiency of (10.4 ± 0.2)% for the ITO/$CuInS_2$/Al_2O_3/$CH_3NH_3PbI_3$/$PC_{60}BM$/Ag cell without CdS.

18/00439 Highly flexible InSnO electrodes on thin colourless polyimide substrate for high-performance flexible $CH_3NH_3PbI_3$ perovskite solar cells

Park, J.-I. *et al. Journal of Power Sources*, 2017, 341, 340–347.

In this study, the authors fabricated high-performance flexible CH3NH3PbI3 (MAPbI3) perovskite solar cells with a power conversion efficiency of 15.5% on roll-to-roll sputtered ITO films on 60 μm-thick colourless polyimide (CPI) substrate. Due to the thermal stability of the CPI substrate, an ITO/CPI sample subjected to rapid thermal annealing at 300 °C showed a low sheet resistance of 57.8 Ω/square and high transmittance of 83.6%, which are better values than those of an ITO/PET sample. Outer and inner bending tests demonstrated that the mechanical flexibility of the ITO/CPI was superior to that of the conventional ITO/PET sample owing to the thinness of the CPI substrate. In addition, due to its good mechanical flexibility, the ITO/CPI showed no change in resistance after 10,000 cycle outer and inner dynamic fatigue tests. Flexible perovskite solar cells with the structure of Au/PTAA/MAPbI3/ZnO/ITO/CPI showed a high power conversion efficiency of 15.5%. The successful operation of these flexible perovskite solar cells on ITO/CPI substrate indicated that the ITO film on thermally stable CPI substrate is a promising of flexible substrate for high-temperature processing, a finding likely to advance the commercialization of cost-efficient flexible perovskite solar cells.

18/00440 Impact of the geometry of divergent chimneys on the power output of a solar chimney power plant

Hu, S. *et al. Energy*, 2017, 120, 1–11.

A divergent chimney is proposed as an alternative for solar chimney power plants (SCPPs) because of their reported remarkable improvement in power output over cylindrical chimneys. However, the power output of divergent SCPPs in those studies changed from several percentage to >100 times higher than that of cylindrical ones. In the authors' hypothesis, this large deviation was related to the various configurations of the SCPPs examined. Therefore, this paper examines comprehensively the effect of geometry of divergent chimneys on system performance of SCPPs to further reveal their hydrodynamic features. The geometric parameters under investigation included the area ratio (AR) of chimney exit over entrance, the divergent angle (DA) of chimney wall and the size of system. The numerical simulations indicated a parabolic tendency in the performance of the divergent SCPPs when increasing the ARs (or DAs). Reasons for this tendency were proposed based on its hydro- and thermo-interaction. Furthermore, the normalized power output showed good consistency among the SCPPs with different sizes when geometric similarity was adopted to the entire system geometry. The similar normalized outputs found were almost insensitive to the variations in the solar insolation. These outcomes would be a valuable reference for designing SCPPs with divergent chimneys.

18/00441 Mass production and modeling of high efficiency n-PERT solar cells with ion implanted BSF/selective-BSF

Shi, J. *et al. Solar Energy*, 2017, 142, 87–90.

Ion implantation is a technique which has already been successfully transferred from integrated circuits (IC) industry to photovoltaic (PV) industry, especially for p-type solar cells fabrication. Based on the configuration of Yingli n-PERT PANDA cells, phosphorus implantation is employed to fabricate n+ back surface field (BSF) as an alternative to $POCl_3$ diffusion. A 20.3% cell efficiency on average with a maximum value of 20.5% was achieved in mass production by process optimization such as ion implantation, annealing during PECVD and passivation improvement. Resulted modelling data indicates that the selective-BSF (SBSF) cell efficiency gain was 0.2% absolute compared with rear totally homogeneous doped cell after process optimization and the SBSF cells reach the best efficiency at a wafer resistivity around 0.5–1 Ω cm depending on wafer lifetime. This study proved that cells with efficiency higher than 21% can be realized by optimizing sheet resistance of rear surface and improving passivation.

18/00442 Modeling of a selective solar absorber thin film structure based on double TiN_xO_y layers for concentrated solar power applications

Zhang, J. *et al. Solar Energy*, 2017, 142, 33–38.

By using double TiN_xO_y absorption layers with low N/O ratio (TiNO_L) and high N/O ratio (TiNO_H), a spectral selective solar absorber (SSA) with the structure of SiO_2-TiO_2-TiNO_L-TiNO_H-Cu has been proposed. Optical properties of the TiNO_L and TiNO_H layers are investigated with spectroscopic ellipsometry (SE) in the wavelength range of 0.3–2.5 μm using an optical dispersion model in which the absorption mechanisms in TiN_xO_y including the localized surface plasmon resonance (LSPR), free electron absorption and interband transitions are taken into account. Because TiNO_H has a higher free electron concentration than that of TiNO_L, the absorption due to both the LSPR and free electron absorption in TiNO_H is found larger than that in TiNO_L. With the model parameters of the dispersion model obtained from the SE modelling, the reflectance spectrum of the SSA in the wide wavelength range of 0.3–25 μm covering both the solar radiation and heat radiation of a hot surface has been simulated; and the simulated result agrees well with the experimental result.

18/00443 Modelling of a Stirling engine with parabolic dish for thermal to electric conversion of solar energy

Barreto, G. and Canhoto, P. *Energy Conversion and Management*, 2017, 132, 119–135.

Stirling engines with parabolic dish for thermal to electric conversion of solar energy is one of the most promising solutions of renewable energy technologies in order to reduce the dependency from fossil fuels in electricity generation. This paper addresses the modelling and simulation of a solar powered Stirling engine system with parabolic dish and electric generator aiming to determine its energy production and efficiency. The model includes the solar radiation concentration system, the heat transfer in the thermal receiver, the thermal cycle and the mechanical and electric energy conversion. The thermodynamic and energy transfer processes in the engine are modelled in detail, including all the main processes occurring in the compression, expansion and regenerator spaces. Starting from a particular configuration, an optimization of the concentration factor is also carried out and the results for both the transient and steady state regimes are presented. It was found that using a directly illuminated thermal receiver without cavity the engine efficiency is close to 23.8% corresponding to a global efficiency of 10.4%. The components to be optimized are identified in order to increase the global efficiency of the system and the trade-off between system complexity and efficiency is discussed.

18/00444 Optimal turbine pressure drop for solar chimney-aided dry cooling system in coal-fired power plants

Li, J. *et al. Energy Conversion and Management*, 2017, 133, 87–96.

In solar chimney-aided dry cooling systems, the low-grade waste heat released by condensers in coal-fired power plants heats the inlet air of solar collectors, thus improves the power output and decreases the power consumption of fans. An analytical model of this hybrid system is proposed to study the characteristics of heat transfer and fluid flow in the water–air heat transfer, solar collector, heat storage layer, draft tower, and turbines. The fitting equation of the optimal turbine pressure drop for the hybrid system is derived, and the effects of the solar collector radius and solar radiation on power outputs are discussed. Results show that the optimal turbine pressure drop is positively correlated to the solar collector radius and solar radiation. However, a critical collector radius and a critical solar radiation for the turbine configuration exist. The performance of a hybrid system integrated with a 660 MW supercritical coal-fired power unit reveals that the optimization scheme proposed in this study outperforms the two schemes provided in the references.

18/00445 Performance analysis of a new high gain dc–dc converter interfaced with solar photovoltaic module

Mitra, L. and Rout, U. K. *Renewable Energy Focus*, 2017, 19–20, 63–74.

This work presents a new single switched high-gain dc–dc converter that can be used in PV systems, in which the low DC output voltage of PV module is converted into high dc output voltage. The proposed converter utilizes a single switch, an inductor and a capacitor to transfer the inductive and capacitive energy simultaneously, achieving a high boost ratio. The voltage gain of the dc–dc converter is obtained as 10. The state space model of the converter is presented and all the performance parameters of the proposed converter are analysed when coupled with a PV module. A practical solar module BPSX150S is designed using manufacturer's datasheet by MATLAB program/.m files. Different MPPT algorithms like P&O, Incremental Conductance and Modified Perturb and Observe algorithm are used to find the maximum power point and extract the maximum power. The complete PV system is modelled using the proposed converter interfaced with the designed PV module with MPPT to keep the output voltage constant. The proposed converter is implemented in hardware for the experimental verifications and the experimental results are presented. All the simulations are done using MATLAB program/.m files and SIMULINK.

18/00446 Performance and financial evaluation of various photovoltaic vertical facades on high-rise building in Malaysia

Ghazali, A. *et al. Energy and Buildings*, 2017, 134, 306–318.

Photovoltaic (PV) façade on building envelope in an urban area can potentially produce clean electricity to meet the energy demand of the buildings and also provide weather protection. In order to assess the potential of PV application on building façade, energy generated and cost related to the PV installation, it must be analysed during the design process so that it can provide enough information to the designer, investor, and end user to make a decision in implementing renewable technologies. This paper focus on performance and financial evaluation using System Advisor Model (SAM) developed by National Renewable Energy Laboratory (NREL) to evaluate the potential of vertical photovoltaic façade system on a high-rise building in Malaysia based on 5 possible design scenario using Heterojunction Intrinsic Thin-film module (HIT-Si) with the nominal efficiency of 15.6%. The annual energy generated through the vertical photovoltaic system is between 400–700 MWh meanwhile roof system generate about 240MWh annually. The payback period for the vertical photovoltaic system in Malaysia is about 12 years. Although the installation of photovoltaic vertical façade in the tropical region can be quite challenging especially in urban area, but with proper studies and carefully design approach, its can open new opportunities in Malaysian built environment.

18/00447 Polyacrylonitrile-grafted reduced graphene oxide hybrid: an all-round and efficient hole-extraction material for organic and inorganic-organic hybrid photovoltaics

Jung, C.-H. *et al. Nano Energy*, 2017, 31, 19–27.

In this research, the authors demonstrate that aliphatic polyacrylonitrile-grafted reduced graphene oxide (PRGO) hybrid can function efficiently as an all-round hole-extraction layer (HEL) in organic and organic-inorganic hybrid perovskite photovoltaic devices (OPVs and

PePVs). The hybrid-structure PRGO was developed by facile and scalable *in situ* radiation-induced reduction and graft polymerization with polymerizable styryl-functionalized graphene oxide and acrylonitrile. The newly developed PRGO exhibits long-term dispersion stability of six months even up to the high concentration of 10 mg/ml. It also shows a full-cover uniform thin-film morphology, good electrical conductivity (0.87 S/cm), high work function (4.87 eV), and excellent weather stability. Moreover, the incorporation of PRGO (as a HEL) into the OPVs and PePVs results in greater efficiency than chemically-converted graphene nanoflakes references, and device durability superior to poly(ethylenedioxythiophene) : poly(styrene sulfonate)-based ones with comparable power conversion efficiencies. Noticeably, the finding demonstrates that the hybrid-structure PRGO provides an all-round and efficient hole-extraction material for use in various conjugated-polymer and perovskite-based photovoltaic systems.

18/00448 Quantifying rooftop photovoltaic solar energy potential: a machine learning approach

Assouline, D. *et al. Solar Energy*, 2017, 141, 278–296.

The need for reduction in CO_2 emissions to mitigate global warming has resulted in increasing use of renewable energy sources. In urban areas, solar photovoltaic (PV) deployment on existing rooftops is one of the most viable sustainable energy resources. This study uses a combination of support vector machines (SVMs) and geographic information systems (GIS) to estimate the rooftop solar PV potential for the urban areas at the commune level (the smallest administrative division) in Switzerland. The rooftop solar PV potential for a total 1901 out of 2477 communes in Switzerland is estimated. Following a six-fold cross validation, the root-mean-square error (also normalized) is used to estimate the accuracy of the different SVM models. The results show that, on average, 81% of the total ground floor area of each building corresponds to the available roof area for the PV installation. Also considering the total available roof area for PV installation, that is, 328 km^2 and roof orientations within $\pm 90^\circ$ of due south, the annual potential PV electricity production for the urban areas in Switzerland is estimated at 17.86 TW h (assumed 17% efficiency and 80% performance ratio). This amount corresponds to 28% of Switzerland's electricity consumption in 2015.

18/00449 Reconfigurable emulator for photovoltaic modules under static partial shading conditions

Mai, T. D. *et al. Solar Energy*, 2017, 141, 256–265.

This paper aims to emulate the *IV* characteristics of a multiple-substring photovoltaic (PV) module under non-uniform irradiance levels by taking into account the breakdown voltage of shaded cells, configurations of bypass diode connections, and cell temperatures. A suitable control scheme for the emulator's power stage significantly improves the performance of the emulator's output. As a result, this PV emulator proves to be capable of performing under various operating conditions of the PV module including uniform irradiation and non-uniform partial shading with great accuracy.

18/00450 Removal of non-CO_2 greenhouse gases by large-scale atmospheric solar photocatalysis

de Richter, R. *et al. Progress in Energy and Combustion Science*, 2017, 60, 68–96.

Large-scale atmospheric removal of greenhouse gases (GHGs) including methane, nitrous oxide and ozone-depleting halocarbons could reduce global warming more quickly than atmospheric removal of CO_2. Photocatalysis of methane oxidizes it to CO_2, effectively reducing its global warming potential (GWP) by at least 90%. Nitrous oxide can be reduced to nitrogen and oxygen by photocatalysis; meanwhile halocarbons can be mineralized by red-ox photocatalytic reactions to acid halides and CO_2. Photocatalysis avoids the need for capture and sequestration of these atmospheric components. Here review an unusual hybrid device combining photocatalysis with carbon-free electricity with no-intermittency based on the solar updraft chimney. Then the authors review experimental evidence regarding photocatalytic transformations of non-CO_2 GHGs. They propose to combine TiO_2-photocatalysis with solar chimney power plants (SCPPs) to cleanse the atmosphere of non-CO_2 GHGs. Worldwide installation of 50,000 SCPPs, each of capacity 200 MW, would generate a cumulative 34 PWh of renewable electricity by 2050, taking into account construction time. These SCPPs equipped with photocatalyst would process one atmospheric volume each 14–16 years, reducing or stopping the atmospheric growth rate of the non-CO_2 GHGs and progressively reducing their atmospheric concentrations. Removal of methane, as compared to other GHGs, has enhanced efficacy in reducing radiative forcing because it liberates more $^{\circ}OH$ radicals to accelerate the cleaning of the troposphere. The overall reduction in non-CO_2 GHG concentration would help to limit global temperature rise. By physically linking greenhouse gas removal to renewable electricity generation, the hybrid concept would avoid the moral hazard associated with most other climate engineering proposals.

18/00451 Self-assembled spectrum selective plasmonic absorbers with tunable bandwidth for solar energy conversion

Zhou, L. *et al. Nano Energy*, 2017, 32, 195–200.

Plasmonic nanostructures enable manipulation of light ranging from ultraviolet, visible to infrared regime based on steering on a variety of optical resonances. For various applications such as biomedical sensing, photodetectors and solar energy conversion, it is desirable to fabricate plasmonic absorbers with finely tuned bandwidth. In this work, for the first time, it is reported that spectrum-selective plasmonic absorbers with flexibly tuned bandwidth can be fabricated by a convenient self-assembly process. The plasmonic absorbers demonstrate an extraordinary absorption (above 90%) with absorption cutoff wavelengths flexibly tuned from visible (~550 nm) to infrared (~2500 nm). The pronounced absorption can be ascribed to plasmon hybridization of the close-packed gold nanoparticles, while optical cut-off effect of the gold-particle-assembly built nanotube leads to the tuneable absorption edge. These tuneable plasmonic absorbers also demonstrate excellent high temperature stability (up to 1073 K) with a thin alumina protection coating and applications for solar steam generation. Therefore, the plasmonic absorbers with tuneable absorption bandwidth and thermal stability can serve as promising candidates for various solar energy conversion applications, such as solar steam generation, photocatalysis, etc.

18/00452 Silver nanowire networks as transparent top electrodes for silicon solar cells

Aurang, P. *et al. Solar Energy*, 2017, 141, 110–117.

Losses caused by the metal top contacts still remain as an issue in crystalline silicon (Si) solar cells. One approach to eliminate shading losses is to utilize transparent nanostructure networks synthesized through rapid and low cost processes. In this work, the potential of highly conductive silver nanowire (Ag NW) networks as transparent top electrodes for the elimination of metallization process in Si solar cells was investigated. Ag NW top contact cells were found to possess enhanced conversion efficiencies with respect to conventional metal contact reference cells. Increase in conversion efficiency was attributed to the elimination of shading losses, preferential scattering of light into the substrate by localized surface plasmon resonances of the Ag NWs and localized and higher charge collection capability with respect to conventional metal contacts.

18/00453 Simultaneously efficient light absorption and charge transport of phosphate and oxygen-vacancy confined in bismuth tungstate atomic layers triggering robust solar CO_2 reduction

Hou, J. *et al. Nano Energy*, 2017, 32, 359–366.

The fundamental catalytic limitations for the photoreduction of CO_2 still remain: low efficiency, poor charge transport and short lifetime of catalysts. To address the critical challenges, an efficient strategy based on spatial location engineering of phosphate (PO_4) and oxygen-vacancy (V_o) confined in Bi_2WO_6 (BWO) atomic layers is employed to establish and explore an intimate functional link between the electronic structures and activities of V_o-PO_4-BWO layers. Both theoretical and experimental results reveal, the V_o-PO_4-BWO layers not only narrow the band gap from the UV to visible-light region but also reduce the resistance. The time-resolved photoluminescence decay spectra exhibit the increasing carrier lifetime for V_o-PO_4-BWO layers, indicating the improved charge separation and transfer efficiency. As expected, the V_o-PO_4-BWO layers with the simultaneously efficient light absorption and charge transport properties achieve much higher methanol formation rate of 157 $\mu mol\ g^{-1}\ h^{-1}$, over 2 and 262 times larger than that of BWO atomic layers and bulk BWO. This work may reveal that the light absorption and spatial charge transport over atomic layers could benefit CO_2 conversion and shed light on the design principles of efficient photocatalysts towards solar conversion applications.

18/00454 Thermal and electrical performance of a hybrid design of a solar-thermoelectric system

Ong, K. S. *et al. Energy Conversion and Management*, 2017, 133, 31–40.

An evacuated tube heat pipe solar collector was fitted with four thermoelectric modules and four water cooling jackets on the condenser side to produce electricity and hot water simultaneously. Each cooling jacket had six mini water-flow channels inside it. Solar heat was absorbed and collected by the evaporator section. Experiments were conducted under outdoor environment with various water coolant flow rates. Once-through coolant water flow was adopted as a first step. Further investigations would be conducted to incorporate an insulated hot water storage tank to evaluate the system economic viability as a power producer and hot water generator. Temperatures were recorded along the evaporator and condenser sections of the heat pipe, thermoelectric junction temperatures and inlet/outlet water channels. This paper presents the experimental results obtained. Typical daily experimental results showed that electrical output voltage

and hot water temperatures peaked around 15.30 before decreasing towards the evening. Total electrical efficiency was very low, about 0.16% at around 15.30 h.

18/00455 Thermal performance of parabolic trough solar collectors

Conrado, L. S. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 1345–1359.

The thermodynamics of a parabolic trough solar collector (PTC) play an important role in solar energy and the efficiency of the collectors. This report presents an up-to-date review on the thermal performance of PTC collectors. Various types of mathematical models, simulation and numerical methods, and experimental set-ups of the PTCs are reviewed. These have been studied in terms of heat loss, environmental conditions, temperature and heat flux. Furthermore, the report cost analysis and economic strategy used for PTC collectors. The primary goal is to demonstrate the principal thermal aspects that need to be considered in future developments. The principal challenges that engineers face are (a) combining the thermal models that have been reported in the literature, (b) introducing numerical methods and simulations with less computational requirements, (c) proposing new methodologies that efficiently measure the thermal performance of a PTCs and (d) reducing the costs of these collectors.

18/00456 Thermochemical energy storage by consecutive reactions for higher efficient concentrated solar power plants (CSP): proof of concept

Cabeza, L. F. *et al. Applied Energy*, 2017, 185, 836–845.

Concentrated solar power plants (CSP) combined with thermal energy storage (TES) offers the benefit to provide continuous electricity production by renewable energy feed. There are several TES technologies to be implemented, being the thermochemical energy storage the less studied and the most attractive since its volumetric energy density is 5 and 10 times higher than latent and sensible TES, respectively. Thermochemical energy storage technology is based on reversible chemical reactions, also named thermochemical materials (TCM). One of the main challenges of TCM is to achieve a proper reversibility of the reactions, which in practical conditions leads to lower efficiencies than the theoretically expected. A new concept based on changing from reversible TCM reactions towards TCM consecutive reactions aims to eliminate reversibility problems and therefore improve the overall efficiency. Consecutive TCM reactions can either be based in one cycle, where reactants are needed to feed the reaction, or two coupled cycles which offer the possibility to work without any extra mass reactants input. The plausibility of the implementation of both concepts in CSP is detailed in this paper and case studies are described for each one.

18/00457 Transient heat extraction modeling method for a rectangular type salt gradient solar pond

Aramesh, M. *et al. Energy Conversion and Management*, 2017, 132, 316–326.

In this article, a transient modelling method for the heat extraction process in the rectangular solar ponds is presented by using a finite difference technique. Firstly, the thermal behaviour of the pond, during the heat extraction operation is modelled. Then the model is verified using experimental data, and the maximum observed percentage error of this method is 2.03%. This method is used to model the heat extraction from a hypothetical pond in Tehran for 3 months of August, September, and November. The results present the temperature profiles, the extracted heat and the rate of heat extraction. All of these parameters have the highest value in August, and the lowest values are allocated to November. Moreover, the percentages of the extracted heat during the operation are studied. For all the 3 months, this parameter has a high value in the first 40% of the time needed to full heat extraction. Between the 40% and 70% of the total time, the heat extraction rate reduces drastically, and after the 70% of the total time, it is almost constant at a low value. Also, the modelling results are used in a low-temperature organic Rankine cycle, and it is found that for the designed pond, the pond can be used as the heat source of the cycle only in August and for 7.31 h of operation.

18/00458 Vacuum pumping options for application in solar thermochemical redox cycles – assessment of mechanical-, jet- and thermochemical pumping systems

Brendelberger, S. *et al. Solar Energy*, 2017, 141, 91–102.

Solar powered two-step thermochemical redox cycles are often investigated as a pathway to producing renewable fuels, via the splitting of water and carbon dioxide. These processes require a high temperature step for the reduction of the redox material. The reduction thermodynamics also critically depend on the oxygen partial pressure. In generic process assessments, purge gases and mechanical vacuum pumps have been considered for removing the released oxygen. Even though both alternatives are expected to have a significant impact on the overall process efficiency, little effort has been made so far in providing a detailed analysis of the implementation of the related components – especially in the case of vacuum pumps. In this study models are developed for assessing the energy requirements of mechanical vacuum pumps as well as for jet pumps. The models are validated and compared to data provided by manufacturers. In addition, a novel thermochemical pumping concept is introduced and a first thermodynamic assessment is presented. The energy demands of the different pump options are discussed in the context of the targeted application. By comparison with the energy stored in the produced fuel, limitations for the implementation of these systems can be identified. Furthermore, the costs for mechanical and jet pumps have been taken into account for the assessment. While mechanical pumps are energetically favoured and could be reasonably applied for pressures down to 150 Pa, jet pumps are the more economic option and can make direct use of waste heat, which should be vastly available in the process at the required temperature level. The concept of thermochemical pumps is energetically very interesting and might shift the limit of realistic operational pressures to lower values, especially when combined with conventional systems.

18/00459 Wind effects on the performance of solar collectors on rectangular flat roofs: a wind tunnel study

Ladas, D. I. *et al. Journal of Wind Engineering and Industrial Aerodynamics*, 2017, 161, 27–41.

Wind induced convection is the main cause of heat loss for roof-mounted solar collectors. In this study the importance of using the actual wind velocity distributions over the whole roof area, instead of a commonly assumed single velocity of a reference location, is addressed through experimental measurements and numerical assessment of the performance of solar collectors placed on different locations over the roof of a typical rectangular building. The measurements were carried out at the Boundary Layer Wind Tunnel of Concordia University, for nine different locations on the roof, three different wind directions and cases concerning both an isolated building and a building with surroundings of various configurations. For the isolated building case, it was found that local velocities on different roof locations may vary more than 60% and the effect of these differences on the performance of solar collectors placed on these locations was assessed. In an attempt to generalize the results, 17 different surrounding configurations were considered. For a typical day in Montreal (with 4–7 m/s average wind speed), it was found that the thermal gains between solar collectors at different locations over the same roof could vary up to 21%.

18/00460 Worldwide analysis of spectral factors for seven photovoltaic technologies

Polo, J. *et al. Solar Energy*, 2017, 142, 194–203.

This work presents a worldwide analysis of the photovoltaic (PV) spectral factor for seven different PV technologies including crystalline silicon and thin film modules. The annual spectral factor for the analysed technologies is evaluated at 124 sites which cover widely the most important climatic zones. This dataset allows determining the spatial and geographical distribution of the spectral gains/losses with respect to reference conditions for the analysed PV technologies. The spectral factors are computed from hourly global tilted spectral irradiances for a whole year using the SMARTS2 spectral solar radiation model with atmospheric inputs from the MACC reanalysis dataset. Overall, it is found that the annual spectral factor for crystalline silicon technologies is rather homogenous worldwide with maxima spectral losses and gains of ≈3% and ≈1%, respectively. The annual spectral factor for thin film devices, on the contrary, displays a latitudinal pattern with spectral losses mainly occurring in northern hemisphere locations and spectral gains occurring in tropical zones. Both spectral gains and losses may reach up to ≈10% in the case of amorphous silicon devices. The correlation analysis between average photon energy (APE) and spectral factor shows high correlation values for thin film devices. However, the data dispersion is large, which discourages the use of APE as a measure of the spectral performance of PV systems.

Wind energy

18/00461 Augmenting DFIG wind turbine transient performance using alternative voltage source T-type grid side converter

Okedu, K. E. *Renewable Energy Focus*, 2017, 18, 1–10.

Voltage source converters (VSCs) are generally used to achieve energy conservation in wind energy applications. The conventional two-level VSCs are commonly used in doubly fed induction generator (DFIG) wind turbines. Recently, the technology of multilevel converters in wind generators is becoming promising compared to the two-level converters. This is because they can overcome some limitations of the

two-level converter performance during transients. This paper presents a new alternative T-type multilevel VSC topology for the grid side converter of the DFIG. The analysis and switching strategy of the T-type converter was presented. Simulations were run in power system computer aided design and electromagnetic transient including DC (PSCAD/EMTDC) and results using the new T-type converter topology were compared with scenarios where the wind generator was protected by conventional crowbar, DC-chopper and parallel interleaved of the two-level converters for the rotor and grid side converters of the DFIG. The results show the improved performance of the wind generator during transient, thus saving the cost of external expensive circuitry (crowbar) and more switching IGBTs (interleaving both converters). Furthermore, the performance of the T-type DFIG based grid converter was enhanced using a braking resistor connected to the stator of the wind generator.

18/00462 Evaluation and comparison of anti-impact performance to offshore wind turbine foundations: monopile, tripod, and jacket

Hao, E. and Liu, C. *Ocean Engineering*, 2017, 130, 218–227.

Offshore wind turbines (OWTs) near shipping lanes are under a potential threat caused by ship impacts during the service period. Contraposing to three common uses of foundations (monopile, tripod and jacket) of offshore wind turbines, this study is devoted to probe and compare the anti-impact performance due to a head-on impact by ships. A series of cases are conducted to investigate the foundation damage and the OWT response of the three types of foundations using LS-DYNA, a commercial FEM tool. Through investigating and analysing the maximum collision force, the damage area, the maximum bending moment of piles at the seabed, the steel consumption and the maximum nacelle acceleration in different low-energy collision scenarios, it is found that the jacket generates the minimum collision force, damage area and nacelle acceleration as well as the medium bending moment and steel consumption among the three. Therefore, the jacket has the optimum comprehensive anti-impact performance under low-energy collisions, which may be useful in developing the foundation design of offshore wind turbines.

18/00463 Grouped grey wolf optimizer for maximum power point tracking of doubly-fed induction generator based wind turbine

Yang, B. *et al. Energy Conversion and Management*, 2017, 133, 427–443.

This paper proposes a novel grouped grey wolf optimizer to obtain the optimal parameters of interactive proportional-integral controllers of doubly-fed induction generator based wind turbine, such that a maximum power point tracking can be realized together with an improved fault ride-through capability. Under the proposed framework, the grey wolves are divided into two independent groups, including a cooperative hunting group and a random scout group. The former one contains four types of grey wolves (i.e. alpha, beta, delta and omega) to accomplish an effective hunting based on their hierarchical cooperation and three elaborative manoeuvres in the presence of an unknown environment, e.g. prey searching, prey encircling and prey attacking, of which the number of beta and delta wolves is increased to achieve a deeper exploitation. On the other hand, the latter one undertakes a randomly global search and realizes an appropriate trade-off between the exploration and exploitation, thus a local optimum can be effectively avoided. Three case studies are carried out which verify that a better global convergence, more accurate power tracking and improved fault ride through capability can be achieved by the proposed approach compared with that of other heuristic algorithms.

18/00464 Is Brazilian wind power development sustainable? Insights from a review of conflicts in Ceará state

Brannstrom, C. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 62–71.

Brazil's wind energy programme is a successful public-private sector response to an electricity supply crisis in 2001 that created an attractive target for investors in renewable power. But evidence is accumulating that environmental impacts, which lead to territorial conflicts, livelihood erosion, and political responses, contradict sustainability claims of wind power development. The authors synthesize conflicts emerging in coastal Ceará state, a pioneer in Brazil's rapid development of wind power. Environmental impacts caused by wind farms, which locate on dune fields and other coastal systems, create conflicts by denying traditional communities access to resources that sustain livelihoods and cultural identities. Resource-access conflicts produce political responses that seek mitigation measures, but may escalate into a wider political challenge to continued development of wind power. This study highlights the importance of land-tenure policies to assure the territorial integrity of traditional communities in areas targeted for wind power implementation. Analysis of conflicts supports suggested solutions for governments, firms, and traditional communities that may be applied in other developing countries and may help investors and planners avoid future conflicts.

18/00465 Lessons from wind policy in Portugal

Peña, I. *et al. Energy Policy*, 2017, 103, 193–202.

Wind capacity and generation grew rapidly in several European countries, such as Portugal. Wind power adoption in Portugal began in the early 2000s, incentivized by a continuous feed-in tariff policy mechanism, coupled with public tenders for connection licenses in 2001, 2002, and 2005. These policies led to an enormous success in terms of having a large share of renewables providing electricity services: wind alone accounts today for ~23.5% of electricity demand in Portugal. The authors explain the reasons that wind power became a key part of Portugal's strategy to comply with European Commission climate and energy goals, and provide a detailed review of the wind feed-in tariff mechanism. They describe the actors involved in wind power production growth and estimate the environmental and energy dependency gains achieved through wind power generation, as well as highlighting the correlation between wind electricity generation and electricity exports. Finally, the authors compare the Portuguese wind policies with others countries' policy designs and discuss the relevance of a feed-in tariff reform for subsequent wind power additions.

18/00466 Modeling of wind turbine wakes under thermally-stratified atmospheric boundary layer

El-Askary, W. A. *et al. Journal of Wind Engineering and Industrial Aerodynamics*, 2017, 160, 1–15.

In this study, the wake behaviour of wind turbines, operating under a thermally stratified atmospheric boundary layer (ABL), is numerically investigated. The steady state three-dimensional Reynolds-averaged Navier–Stokes (RANS) equations, combined with the actuator disk approach, are used in the simulation. The standard k–ε turbulence model as well as a modified one namely El Kasmi model are adopted. Two different methods are used and compared, for representing the atmospheric stratification flow conditions: In the first one (direct method), the energy equation is considered along with mass, momentum, and turbulence model equations. In the second one (indirect method), stratification is modelled by means of additional buoyancy production and dissipation terms. Such terms are added to the turbulent kinetic energy and dissipation rate equations, instead of solving the energy equation. The results obtained from both methods show a reasonable agreement with the experimental data available from the literature. Moreover, it is concluded that, there is no significant difference between the predicted results from both methods. Further, the effect of the atmospheric stability class on the wake deficit and the available wind power in the wake region has been also investigated using the indirect method. It was found that there is a significant influence of the different atmospheric conditions on the wake behaviour. In particular, the wake region becomes smaller with the decreasing of atmospheric stability, and hence a higher wind power in the wake region is observed for unstable conditions.

18/00467 Multi-criteria selection of offshore wind farms: case study for the Baltic States

Chaouachi, A. *et al. Energy Policy*, 2017, 103, 179–192.

This paper presents a multi-criteria selection approach for offshore wind sites assessment. The proposed site selection framework takes into consideration the electricity network's operating security aspects, economic investment, operation costs and capacity performances relative to each potential site. The selection decision is made through analytic hierarchy process (AHP), with an inherited flexibility that aims to allow end users to adjust the expected benefits accordingly to their respective and global priorities. The proposed site selection framework is implemented as an interactive case study for three Baltic States in the 2020 time horizon, based on real data and exhaustive power network models, taking into consideration the foreseen upgrades and network reinforcements. For each country the optimal offshore wind sites are assessed under multiple weight contribution scenarios, reflecting the characteristics of market design, regulatory aspects or renewable integration targets.

18/00468 Multi-objective differential evolution optimization based on uniform decomposition for wind turbine blade design

Wang, L. *et al. Energy*, 2017, 120, 346–361.

Wind turbine blade design is a complicated multi-objective optimization task. In this article, a novel gradient-based multi-objective evolution algorithm based on both uniform decomposition and differential evolution is proposed for the design of wind turbine blades, to overcome unsatisfactory convergence performance and diversity of solutions usually existing in conventional evolution algorithms. A uniform decomposition mechanism is developed to achieve homogeneous discretion of the objective space for the purpose of controlling population distribution. Meanwhile, a differential

evolution mechanism based on neighbourhood and gradient is developed to achieve exploration-exploitation balance and enhance optimization efficiency of the algorithm proposed. Two-objective, three-objective, and four-objective optimizations for the 1.5 MW wind turbine blade designs reveal that the proposed algorithm exhibits improved distribution, convergence, and converging efficiency compared to the conventional evolution algorithms such as NSGA-II. Additionally, the improvements are more significant with more objectives involved, demonstrating that the proposed algorithm can serve as a universal, high performance algorithm for the multi-objective optimization of wind turbine blade design.

18/00469 Multivariate optimization of off-grid wind turbines with variable demand – case study of a remote commercial building

Baniassadi, A. *et al. Renewable Energy*, 2017, 101, 1021–1029.

Generally, in optimization of wind turbines, the annual energy output is set as the objective function. However, as verified in this study, maximizing the annual energy does not necessarily guarantee the optimum design for off-grid wind turbines. In such cases, the demand profile can have a significant effect on design and performance of the rotor. In this study, an off-grid wind turbine is optimized while considering the demand profile. Blade element method, genetic algorithm, and EnergyPlus are applied in a coupled scheme to obtain the optimum design. Results suggest that if minimizing the annual energy deficit or fuel consumption is set as the objective function, the obtained optimum design will be different to the case in which maximizing the annual wind generated energy is set as the target. Accordingly, in the investigated case of this study, the annual wind fraction increased up to 5% by applying the proposed objective function.

18/00470 Nonlinear short term extreme response of spar type floating offshore wind turbines

Aggarwal, N. *et al. Ocean Engineering*, 2017, 130, 199–209.

In this work, the dynamic characteristics of spar based floating 5 MW offshore wind turbine (OWT) are studied under operational and survival conditions for offshore Indian conditions. The spar with OWT is installed in 320 m water depth. The OWT is subjected to combined wind and wave loads according to irregular Pierson–Moskowitz spectrum. After obtaining non-linear spar platform responses, 3-h short term extreme motions are calculated which are useful for the design of an OWT. Extreme values provide realistic estimates to the associated risk of an event since the tail region governs the largest/smallest events or even the events over a threshold in a sample. In this paper, the extreme values are obtained by fitting the peaks in the tail regime using a Weibull-distribution. While one obtains Gaussian responses under the survival loads, the operational conditions have non-Gaussian responses and also larger than survival ones. The results show one should exercise caution for generating the extreme values for non-Gaussian responses and do a proper sensitivity analysis with respect to samples used for generation of extremes.

18/00471 Optimizing the number and locations of turbines in a wind farm addressing energy-noise trade-off: a hybrid approach

Mittal, P. *et al. Energy Conversion and Management*, 2017, 132, 147–160.

Micro-siting is an optimal way of placing turbines inside a wind farm while considering various design objectives and constraints. Using a well-established Jensen wake model and ISO-9613-2 noise calculation, this study performs a wind farm layout optimization based on a multi-objective trade-off between minimization of the noise propagation and maximization of the energy generation. A novel hybrid methodology is developed which is a combination of probabilistic real-binary coded multi-objective evolutionary algorithm and a newly proposed deterministic gradient based non-dominated normalized normal constraint method. Based on the Inverted Generational Distance metric, the performance of the proposed method is found to be better than the conventional normalized normal constraint method or the concerned evolutionary method alone. Moreover, in contrast to the previous studies, the generated non-dominated front is capable of providing a trade-off between various alternative energy-noise solutions, along with an additional information about the corresponding turbine numbers and their optimal location coordinates. As a result, the decision maker can choose from different competing wind turbine layouts based on existing noise and other standard regulations.

18/00472 Performance characteristics of a horizontal axis turbine with fusion winglet

Zhu, B. *et al. Energy*, 2017, 120, 431–440.

Any technique or method that can improve the efficiency in exploiting renewable wind or marine current energy has got a great significance today. It has been reported that adding a winglet at the tip of the rotor blades on a horizontal axis wind turbine can increase its power performance. The purpose of this paper is to adopt a numerical method to investigate the effects of different winglet configurations on turbine performance, especially focusing on the direction for the winglet tip to point towards (the suction side, pressure side or both sides of the main blade). The results show that the new design of an integrated fusion winglet proposed in this paper can generally improve the main blade's power producing ability, which is further enhanced with the increase of turbine's tip speed ratio with a maximum power augmentation of about 3.96%. No matter which direction the winglet tip faces, the installation angle of the winglet should match well with the real angle of incoming flow. As a whole, the turbine with winglet of two tips facing to both sides of the main blade can produce much more power than the one of winglet configuration whose tip faces only one side for different blade hub pitch angles and vast majority of tip speed ratios. The working principle behind the winglet in improving turbine performance may be that it can block the downwash fluid easily flowing around the tip section of the main blade from the pressure side to suction side, and hence diffuse and spread out the tip vortex. As a result, it finally decreases the energy loss. Besides, the relative projected rotor area in incoming flow direction will also be reduced due to the addition of the winglet, which is also helpful to turbine's power coefficient.

18/00473 Scaling of slow-drift motion with platform size and its importance for floating wind turbines

Lupton, R. C. and Langley, R. S. *Renewable Energy*, 2017, 101, 1013–1020.

Slow drift is a large, low-frequency motion of a floating platform caused by non-linear hydrodynamic forces. Although slow drift is a well-known phenomenon for ships and other floating structures, new platforms for floating wind turbines are significantly smaller in scale, and it is yet to be established how important slow drift is for them. This paper derives an approximate expression for the scaling of the slow drift motion with platform size, mooring characteristics and wave conditions. This suggests that slow drift may be less important for floating wind turbines than other, larger, floating structures. The accuracy of the approximations is discussed; in the one case where detailed data is available, the approximate result is found to be conservative by a factor of up to 40.

18/00474 Short-term wind power prediction based on spatial model

Ye, L. *et al. Renewable Energy*, 2017, 101, 1067–1074.

Large-scale integration of wind energy into power systems may cause operational problems due to the stochastic nature of wind. A short-term wind power prediction model based on physical approach and spatial correlation is proposed to characterize the uncertainty and dependence structure of wind turbines' outputs in the wind farm. Firstly, continuous partial differential equation of each wind turbine has been developed according to its specific spatial location and the layout of its neighbouring correlated wind turbines. Then, spatial correlation matrix of wind speed is derived by discretizing differential equation at each wind turbine using a finite volume method. Wind speed at each turbine is acquired by solving the relevant differential equation under given boundary conditions. Finally, the wind speed is converted to wind power production via a practical power curve model. Prediction results showed that the spatial correlation model can accurately characterize the correlations among outputs of wind turbines and reduce the error of short-term wind power prediction.

18/00475 Wind generation's effect on the *ex post* variable profit of compressed air energy storage: evidence from Texas

Liu, Y. *et al. Journal of Energy Storage*, 2017, 9, 25–39.

This study used 1401 daily observations in the 46-month period of 1 January 2011 to 31 October 2014 to estimate the effect of wind generation on the daily per MWH arbitrage profits of compressed air energy storage (CAES) in the four regions of Houston, north, south and west in the Electricity Reliability Council of Texas (ERCOT). It was found that an increase in wind generation's MWh output in the discharge hours tended to reduce a CAES system's profits. The same MWH increase in the charge hours, however, tended to increase profits. Hence, a wind generation capacity expansion that increases wind MWh in both discharge and charge hours has offsetting profit effects, implying that a CAES unit's profitability is unlikely affected by wind generation development. Sharply contrasting the 'gone with the wind' profitability problem faced by natural-gas-fired generation, these findings lend support to the financial attractiveness of CAES, whose development is useful for integrating a rising share of wind generation capacity into an electric grid.

Others, including economics

18/00476 A CFD presentation and visualization for a new model that uses interceptors to harness hydro-energy at the wash of fast boats

Talaat, W. M. *et al. Ocean Engineering*, 2017, 130, 542–556.

This paper proposes a scheme for harnessing flow energy downstream of the propeller of boat, using a perforated interceptor plate. The proposed scheme is the first of its kind, which is thought to provide electrical energy if applied on board fast boats. Mainly, the authors study a model composed of an elbow piping set that is connected to a perforated interceptor plate, constituting the inlet configuration (or the penstock) to water turbine. A commercial computational fluid dynamics tool was essentially implemented to predict the model's initial gain and to present some of the important fluid dynamics aspects of the problem. They studied the flow upstream of the proposed model of interceptor and illustrated the effects of the upstream external flow and the boundary layer on the flow through the piping bends and downstream. As expected, the traditional interceptor model is majorly affected by the modelled perforations. Hence, the performance of the perforated interceptors was investigated. A remarkable flow structure in the developing and fully developed regions of the model was depicted. Finally, the authors reached at some conclusions about the impact on ship performance and the possible measures that may increase the energy gain in the future.

18/00477 A conceptual framework for the analysis of the effect of institutions on biofuel supply chains

Moncada, J. A. *et al. Applied Energy*, 2017, 185, 895–915.

The economic performance of biofuels supply chains depends on the interaction of technical characteristics as technological pathways and logistics, and social structures as actor behaviour, their interactions and institutions. Traditional approaches focus on the technical problems only. Little attention has been paid to the institutional analysis of biofuel supply chains. This paper aims to extend the analysis of the effect of institutions on the emergence of biofuel supply chains by developing a conceptual framework that combines elements of complex adaptive systems, (neo) institutional economics and socio-technical systems theory. These elements were formalized into an agent-based model. The proposed method is illustrated by a case study on a biodiesel supply chain in Germany. It was found that the patterns in production capacity result from investors basing their decisions on optimistic perceptions of the market development that increase with a favourable institutional framework. Conversely, patterns in biodiesel production cannot be completely explained by this mechanism. The proposed framework assisted the model conceptualization phase and allowed the incorporation of social structures into the agent-based model. This approach could be developed further to provide insights on the effect of different future deployment strategies on bioenergy systems emergence and development.

18/00478 A study on a novel two-body floating wave energy converter

Dai, Y. *et al. Ocean Engineering*, 2017, 130, 407–416.

This paper proposes a novel wave energy converter (WEC), which is needed for monitoring the marine environment. The converter is composed of two oscillating bodies: a floating sphere connected to a heavy submerged sphere using a tight rope and a power take off (PTO) system mounted in the floater. Energy is converted from the relative motion between the differently oscillating bodies caused by the action of the waves. The model was first tested in the frequency domain to optimize the geometry and mechanical parameters, and subsequently, a time domain model was built for simulation of a multi-DOF motion system. In the frequency domain research, a constraint was first added to the two-body WEC to address the problem of the small value of the optimized PTO damping. The state space approximation method was employed during the time domain simulation, and external forces acting on the bodies due to the tight rope were deduced. The motions of the system and power absorbed by the converter under regular and irregular waves were analysed in detail. Finally, experiments were conducted on a scaled model, and the results show that the total power efficiency was more than 20%.

18/00479 Assessment of bioenergy development potential and its environmental impact for rural household energy consumption: a case study in Shandong, China

Jiang, Z. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 1153–1161.

The status and changes of the rural household energy consumption (RHEC) and its pollutants emission in Shandong province, China, from 1995 to 2010 were assessed, as well as the reductions of the air pollutants by developing modern bioenergy (MBE). The results indicated that the RHEC significantly increased with annual growth rate of 1.04% during the study period, and significantly changed from the traditional energy use pattern to the commercial energy use pattern. The income effect (ΔRE^t_{ri}) was identified as the critical factor responsible for the increased RHEC, while the energy intensity effect (ΔRE^t_{ei}) and the population effect (ΔRE^t_{rp}) were the dominant factors responsible for the decreased RHEC. Correspondingly, total emissions of the majority pollutants including CO_2, particulate matters (PMs), NO_x and SO_2 significantly increased with increasing RHEC, and positively correlated with the proportion of commercial energy (*PCE*) used in RHEC ($r = 0.821$–0.992, $P < 0.05$). In addition, CO emission showed a slight decreasing tendency in the same period. Based on the status of RHEC in 2010, the total development potential of MBE can reach up to 11.0×10^6 tce, thus the emissions of CO_2, CO, PMs and SO_2 can be reduced by 64.8%, 90.6%, 78.7% and 64.2%, respectively. Unfortunately, the emission of NO_x will increase by 31.8%, which is mainly due to the biomass-fired electricity rather than the coal-fired electricity. These results indicated that multiple benefits could be achieved through using the CS feedstock to develop the MBE products for RHEC.

18/00480 Comparative analysis of different wave turbine designs based on conditions relevant to northern coast of Egypt

Shehata, A. S. *et al. Energy*, 2017, 120, 450–467.

Wave energy has a great potential to solve the unrelenting energy deficiency in Egypt. The present work recommends Wells turbine as a suitable choice for the Egyptian coasts due to its simple and efficient operation under low input air flow. In addition, the possibility of extracting the wave energy from the Egyptian coasts was investigated using the oscillating water system based on real data from the site. To achieve this purpose, two-dimensional numerical models for Wells turbine airfoils, functioning under sinusoidal wave flow conditions, were built. Moreover, the running and starting characteristics under sinusoidal-flow conditions were investigated using a mathematical code. The results were discussed using the first law analysis, in addition to the second law analysis by using the entropy generation minimization method. It was found that the NACA0015 airfoil always gives a global entropy generation rate that is less than other airfoils by approximately −14%, −10.3% and −14.7% for the sinusoidal wave with time periods equal to 4, 6 and 8 s respectively. Moreover, the effects of blade profile, time period and solidity on the output power (kW) value were discussed.

18/00481 Comparison of numerical and experimental analyses for optimizing the geometry of OWC systems

Mahnamfar, F. and Altunkaynak, A. *Ocean Engineering*, 2017, 130, 10–24.

There is a considerable amount of wave energy that can be extracted from the oceans. This energy is largely untapped. The oscillating water column (OWC) is a mechanical system that utilizes fluctuating water level from sea waves to drive an air turbine which, in turn, provides electricity when transmitted to a generator. In this study, two sets of modelling, each involving a numerical modelling and a physical experimental modelling, were conducted in a wave flume to optimize OWC systems. By varying the length, width and angle of the air chamber, an OWC structure can be designed to obtain the maximum system power. The data used for designing the optimal geometry of the chamber that may yield the maximum conversion of wave energy to useful energy were provided from the interpretation of the measurements of these parameters. In this study, results of the numerical models were compared with the measured experimental values based on the Nash–Sutcliffe coefficient of efficiency (NSE) as performance evaluation criterion. The NSE values of both the classical and the modified OWC structures were obtained to be 0.97. It is observed that the results of the numerical models tend to follow much closer the results of the experimental model.

18/00482 Contribution of tidal power generation system for damping inter-area oscillation

Mehri, S. *et al. Energy Conversion and Management*, 2017, 132, 136–146.

The growing need for the clean and renewable energy has led to the fast development of grid-connected tidal stream power generation systems all over the world. These large scale tidal stream power generation systems are going to be connected to power systems and one of the important subjects that should be investigated is its impacts on power system stability. Hence, this paper investigates the possibility of tidal stream power generation system on damping inter-area oscillations, as a new contribution to earlier studies. As tidal farms are mostly installed far from conventional power plants, local signals do not include good quality to alleviate inter-area oscillations. To overcome the problem, a novel damping controller is developed by employing wide-area measurement system and added to base controllers of doubly-fed induction generator through tidal stream power generation system. The proposed wide-area damping controller

includes efficient means to compensate for the incompatible performances of wide area measurement based delayed signals. Robustness of the designed damping controller has been demonstrated by facing the study system with faults leading to enough shifts in power system operating point, and tidal farm generation.

18/00483 Control, power and electrical components in wave energy conversion systems: a review of the technologies

Ozkop, E. and Altas, I. H. *Renewable and Sustainable Energy Reviews*, 2017, 67, 106–115.

The purpose of this paper is to introduce the status of wave energy conversion (WEC) technologies from a different perspective. Past studies based on WEC systems are summarized and classified in terms of WEC system components to clearly reveal the performance, efficiency and development of WEC technologies over the last two decades. It has been proved that the individual components of a WEC system, such as types of wave energy converter and generator motion, control methods and power electronic converter, have a close relationship with each other and that no single component can be optimized without considering the others. It can be helpful to divide into descriptive parts to provide a better understanding of the development process for WEC technologies so that studies based on WEC technologies are discussed by regarding types of wave energy converters, generators, control methods, controller applied sides, waves, power electronic converters and validations and publication year in this paper.

18/00484 Dams turning devils: an insight into the public safety aspects in operational run of the river hydropower projects in western Himalayas

Kumar, D. and Katoch, S. S. *Renewable and Sustainable Energy Reviews*, 2017, 67, 173–183.

A large number of run of the river (RoR) hydropower projects have been planned in hydro rich western Himalayan region. However, public safety aspects are not given due consideration during operation of these projects and many people had lost their lives in the recent past. This study aims at reviewing public safety norms/aspects in these regions and suggests suitable safety measures. Qualitative approach has been adopted to study the problem in detail by undertaking a case study in Himachal Pradesh, a western Indian Himalayan hydro rich state. The study concludes that there is an urgent need to develop and effectively implement public safety standards and/or manuals for operation of RoR hydropower projects in the region under study. The study may be useful in creating awareness and framing of imperative public safety norms for operational RoR hydropower projects in western Himalayan region of India and similar other regions across the world.

18/00485 District heating systems based on low-carbon energy technologies in Mediterranean areas

Lizana, J. *et al. Energy*, 2017, 120, 397–416.

Heating and cooling are responsible for 70% of energy consumption in European buildings, with renewables covering only 18%. To reduce emissions in the building sector, district heating based on low-carbon energy is identified as a key technology for the transition to a low-carbon economy. However, currently only 16% of thermal district networks are based on biomass, and around 3.2% on solar. This paper analyses the application of solar and biomass district heating systems in the low-to-moderate population density areas of the Mediterranean. These areas are characterized by high solar and biomass availability, and lack of space restrictions, along with particular challenges for implementation. A methodology for viability analysis and optimized integration is presented. The methodology is applied to a case study in the south of Spain. The results show that with a linear heat density greater than 1.5 MWh/m, there could be viability with internal rates of return higher than 7.4 and 9.8%, and payback period below 13 and 10 years, for solar and biomass systems, respectively. The use of seasonal thermal energy storage allows the solar fraction to be increased from 55 to 75%. Sizing and design strategies for their viable implementation in Mediterranean areas are extrapolated from the analyses.

18/00486 Economic analysis and environmental impact of flat plate roof mounted solar energy systems

Michael, J. J. and Selvarasan, I. *Solar Energy*, 2017, 142, 159–170.

The flat plate solar water heating system and solar photovoltaic (PV) system are two mature technologies available in the commercial market, which can decrease the residential energy requirement substantially. Several research organizations are working on solar PV/T system to make it competitive to solar thermal system and solar PV system. Innovative designs over the decades have improved the performance of the solar PV/T collector significantly. However, the choice of material-of-construction play a vital role in reducing the mass, cost, embodied energy and embodied CO_2 emissions of the solar PV/T collector. In this paper, a solar PV/T based water heating system was compared with a solar PV system and a flat plate solar water heating (SWH) system based on economic evaluation and environmental assessment. Results obtained show that due to the higher overall efficiency, the solar PV/T system has better benefit-to-ratio compared to solar PV system, while being competitive to solar thermal system. Also, it makes the best use of the available domestic roof-space, minimizes quantity of construction materials and payback period. Further, the embodied energy and embodied CO_2 emission of the PV/T collector is less than the other two solar energy systems combined.

18/00487 Economic and environmental assessment of agro-energy wood biomass supply chains

Paolotti, L. *et al. Biomass and Bioenergy*, 2017, 97, 172–185.

The aim of this study is to conduct an economic and environmental assessment of forest biomass for heating, in particular two types of firewood and three types of wood chips were analysed. Regarding economic aspects, an analysis was made of production costs and revenues (per tonne of biomass), considering all the stages involved 'from the woods to the mouth of the boiler'. For the environmental analysis, conducted using life cycle assessment, the stages taken into account went from 'the woods to the heat produced'. The wood biomasses were compared to each other and to fuel oil and natural gas. The economic analysis showed that at current market prices it is more profitable to produce firewood rather than wood chips. As concerns the environmental aspects, the results of the LCA showed that, for the same heat output, forest wood-based fuel has an environmental impact lower than fuel oil, but still higher than natural gas. There are no big differences in the impact of various wood fuels. In the conclusion, some ways for improvement have been proposed, in terms of both the economic competitiveness of the agro-energy supply chains considered and the reducing of their environmental impact.

18/00488 Evaluation of biomass energy potential towards achieving sustainability in biomass energy utilization in Sabah, Malaysia

Suzuki, K. *et al. Biomass and Bioenergy*, 2017, 97, 149–154.

The potential of biomass energy in Sabah, Malaysia was analysed by data which were established from literature, statistic data and available documents for estimating the potential of biomass energy derived from oil palm, coconut shell, rice, livestock and forest. Nowadays, the issue of solid biomass residues including effluent from the palm oil milling process has become a big concern for the industry and the public in Sabah, because oil palm residues provide a huge potential of biomass energy in Sabah. This paper showed that biomass energy potential in Sabah was around 267,179,818 GJ/year in total, which was derived from oil palm empty fruit bunches, shell, oil palm frond, oil palm trunk, coconut shell, rice, livestock and forest. Potential of biomass energy from oil palm, coconut shell, rice, livestock and forest was 263,635,079, 95,713, 710,028, 750,696 and 1,988,301 GJ/year, respectively. Most biomass energy came from oil palm, which was around 98.7% of total potential. If this total energy potential is applied at a power plant with efficiency ratio of 25% and 8000 h per year of operation, this has potential of 2288 MW, which is equivalent to around 3.8 times the total supply of electricity in 2010 in Sabah. This paper also suggests that relevant policy and innovative technology be developed based on the result to effectively utilize biomass.

18/00489 Feasibility study of energy storage by concentrating/desalinating water: concentrated water energy storage

He, W. and Wang, J. *Applied Energy*, 2017, 185, 872–884.

The paper is to report the work on a preliminary feasibility study of energy storage by concentrating/desalinating water. First, a novel concentrated water energy storage (CWES) is proposed which aims to use off-peak electricity to build the osmotic potential between water bodies with different concentrations, namely brine and freshwater. During peak time, the osmotic potential energy is released to generate electricity. Two scenarios of CWES are specified including a CWES system using reverse osmosis (RO) and pressure retarded osmosis (PRO), and a CWES system co-storing/generating energy and freshwater using 'osmotic-equivalent' wastewater. A comprehensive case study is carried out with focusing on the configuration of CWES using RO and PRO. It is found that the limiting cycle efficiency of the CWES using RO and PRO is inversely proportional to the RO water recovery and independent of the initial salinity. Therefore, to balance the energy density and cycle efficiency of CWES, it is recommended to operate a system at lower RO water recovery with higher concentration of the initial solution. Detailed energy analysis of detrimental effects in mass transfer, e.g. concentration polarization and salt leakage, and energy losses of pressurization and expansion of pressurized water, are studied. Finally, a preliminary cost analysis of CWES is given.

18/00490 Financial attractiveness of decentralized renewable energy systems – a case of the central Himalayan state of Uttarakhand in India

Yaqoot, M. *et al. Renewable Energy*, 2017, 101, 973–991.

Financial viability is arguably the most important requirement for large scale dissemination of decentralized renewable energy systems (DRESs). Financial viability of a DRES can vary from region to region as it depends on various geographical and socio-economic factors. With sufficient solar radiation availability throughout the year, abundant forest cover, dependence of majority of population on agriculture and remote villages facing energy access related challenges, the state of Uttarakhand in India has significant potential for the application of solar and biomass based DRESs. Based on the current fuel prices, subsidies and rebates, this study is an attempt to assess the financial attractiveness of solar and biomass based DRESs under various scenarios for their potential users in Uttarakhand. Improved biomass cookstove, domestic solar water heater, solar lantern and solar home system are found to be financially viable under almost all scenarios for household applications while dish type solar cooker, solar PV pump and solar dryer are not so attractive for household applications. It has also been found that the financial attractiveness of DRESs improve significantly with the removal of subsidy presently being given to fossil fuel based energy supply options.

18/00491 Green in the heart or greens in the wallet? The spatial uptake of small-scale renewable technologies

Allan, G. J. and McIntyre, S. G. *Energy Policy*, 2017, 102, 108–115.

The introduction of a feed-in-tariff (FIT) support mechanism has spurred development of small-scale domestic renewable electricity generation throughout Britain, however the spatial pattern of uptake has been uneven, suggesting that local, as well as between neighbourhood, factors may be at important. As well as confirming that local socio-economic factors, including wealth, housing type and population density are found to be important in explaining uptake of this policy, local 'green' attitudes – measured in three different ways – are shown not to be important. Existing local technical expertise, proxied for using data on small-scale renewable electricity devices in each area prior to the introduction of FIT, is an important factor in explaining subsequent adoption. Critically, it was also found that there are spatial (i.e. between neighbourhood) processes explaining the uptake of these technologies. Taken together, these results suggest that, as currently designed, FIT policy may be regressive in income and could exacerbate spatial economic inequalities.

18/00492 Hydrodynamic performance evaluation of a wave energy converter with two concentric vertical cylinders by analytic solutions and model tests

Cho, I. H. and Kim, M. H. *Ocean Engineering*, 2017, 130, 498–509.

In this paper, the hydrodynamic performance of a two-concentric-cylindrical-body wave energy converter (WEC) is investigated through a systematic parametric study by using analytical solutions and model tests. The two-body WEC generates power by linear electric generator (LEG) through the relative heave motion between the inner and outer buoys. In order to maximize the relative heave motions between the two buoys, resonance of each buoy was used. As a means of finding its maximum hydrodynamic efficiency, the matched eigenfunction expansion method was applied to obtain the analytic solutions under the assumption of linear potential theory. The numerical results are validated through comparisons with a series of model tests conducted by authors in a 2-D wave tank at Jeju National University. Based on the case study, several design strategies that can further enhance the power take-off (PTO) efficiency are proposed, including the optimal PTO damping and intentional mismatching of heave natural frequencies of the two buoys and the peak frequency of target wave spectrum. The intentional mismatching strategy, in particular, can increase high-quality extracted power for broader wave conditions, which is a big advantage in designing the proposed WEC–LEG system.

18/00493 Hydroelectric generator from transparent flexible zinc oxide nanofilms

Li, X. *et al. Nano Energy*, 2017, 32, 125–129.

Harvesting wave energy based on waving potential, a newly found electrokinetic effect, is attractive but limited mainly to monolayer graphene. Here the authors demonstrate that moving a transparent flexible ZnO nanofilm across the surface of ionic solutions can generate electricity. The generated electricity increases linearly with the moving velocity with an open-circuit voltage up to tens of millivolt and a short-circuit current at the order of microampere. The harvested electricity can be efficiently scaled up through series and parallel connections. Theoretical simulations show that it is the proper electrical property that endows the ZnO nanofilm with the outstanding capacity in harvesting the wave energy.

18/00494 Influence of the power take-off characteristics on the performance of CECO wave energy converter

López, M. *et al. Energy*, 2017, 120, 686–697.

Previous experimental works proved the ability of CECO, a wave energy converter (WEC), to harness wave energy. This WEC is presently at technology readiness level (TRL) 3, where characterizing the energy conversion stages and evaluating the energy conversion efficiency is crucial. Therefore, in this work Ansys Aqwa was applied to study a CECO unit and to obtain a detailed knowledge of its performance throughout the different energy conversion stages. The numerical model was initially calibrated with results from experimental tests and then used to simulate different configurations of the power take-off (PTO) system under a wide range of regular and irregular wave conditions. For most of the irregular wave conditions tested, CECO can absorb between 10% and 40% of the incident wave power and transmit to the electric generator up to 18%. Although the results reveal a high-energy conversion efficiency, there is still scope for improvement of the device by optimizing the PTO. On these grounds, the ideal values of the electric generator damping coefficient are presented for different wave conditions, which allow to define an adequate control strategy in future works.

18/00495 Integrated triboelectric nanogenerator array based on air-driven membrane structures for water wave energy harvesting

Xu, L. *et al. Nano Energy*, 2017, 31, 351–358.

Water wave energy is considered a promising renewable energy source, while currently little has been exploited due to a number of unsolved challenges for present technologies. The triboelectric nanogenerator (TENG), as an emerging energy harvesting technology, shows particular advantages in transforming low frequency mechanical energy into electricity, providing new opportunities for harvesting water wave energy. In this work, an integrated triboelectric nanogenerator array device based on air-driven membrane structures is demonstrated. With novel designs of a spring-levitated oscillator structure and a mechanism to use air pressure to transfer and distribute harvested water wave energy, the device can drive a series of integrated TENG units effectively and simultaneously. While operating at low frequency near the resonant frequency of about 2.9 Hz, the device integrating 38 TENG units shows high output of transferred charges per cycle of 15 μC, short-circuit current of 187 μA and optimized peak power density of 13.23 $W m^{-3}$. The device can easily integrates large-scale high-density TENG arrays in one package, as can greatly augment the output, providing a promising route to effectively harvest water wave energy for various practical applications.

18/00496 Levelized cost of energy modeling for concentrated solar power projects: a China study

Zhao, Z.-Y. *et al. Energy*, 2017, 120, 117–127.

Renewable energy plays significant role in achieving energy savings and emissions reduction. As a sustainable and environmental friendly renewable energy source, concentrated solar power (CSP) is of interest for research and development. This is because CSP plants can be equipped with thermal storage systems, thereby producing electricity when sunlight is not available. The installation of CSP plants also leads to substantial 'peak shaving effects'. However, the cost of CSP generation is an obstacle hampering the commercialization of this emerging industry. This paper constructs a mathematical model of the levelized cost of energy (LCOE) to calculate the power generation cost of CSP projects on the basis of lifetime cost structure analysis. A sensitivity analysis is conducted to examine the impact of different variables on the LCOE of CSP projects. The variables considered in this study are investment cost over the construction period, annual operation and maintenance cost, annual electricity production and the discount rate. Finally, the influence of incentive policies such as preferential loans, tax support and zero land cost for power stations is analysed. This research offers a new method for power generation cost calculation of CSP projects and provides support for governments to formulate incentive policies for the industry.

18/00497 Local community as shareholders in clean energy projects: innovative strategy for accelerating renewable energy deployment in India

Thapar, S. *et al. Renewable Energy*, 2017, 101, 873–885.

The Indian government is promoting renewable energy sector with an ambitious target of 175 GW capacity, to be achieved by 2022. The reasons for this energy transition from fossils to renewable energy technologies include facilitating energy access, promoting cleaner forms of energy and enhancing energy security. The huge capacity shall require about 200,000 ha of land. However, land procurement has been identified as a key impediment in accelerating the growth of renewable energy sector in India. This presents an exciting business opportunity towards setting up community energy projects under community mode with the local people as shareholders. Community members can provide their land for setting up renewable energy

projects as well as support in project development activities in lieu of getting up to 15% equity participation. This shall provide them with a constant source of income, estimated at over US$4000 per hectare per annum, besides facilitating energy access in villages. Quicker possession of land shall expedite project execution and the reduced capital expenditure shall decrease the cost of energy generation by up to 6%. Policy makers in emerging economies like India can pilot the proposed model in upcoming solar parks and wind farms.

18/00498 Long-term analysis of wave power potential in the Black Sea, based on 31-year SWAN simulations

Akpinar, A. *et al*. *Ocean Engineering*, 2017, 130, 482–497.

This study analyses the wave energy potential in the Black Sea based on long-term model simulations. A dataset covering the period of 1979–2009 is produced using a calibrated numerical wave prediction model (SWAN). This dataset was analysed in detail to determine the wave energy potential to enable a reliable and optimal design of wave energy conversion devices in the Black Sea. This analysis provides information on the long-term variability as well as on the annual, seasonal and monthly averages. The analysis of the hindcast results is conducted on a spatial and a location scale. The spatial analysis provides information for the entire Black Sea on; the averaged mean wave energy flux over the period 1979–2009, and the decades 1980–1989, 1990–1999, and 2000–2009, seasonal and monthly averages of wave energy flux during 31 years, variability indices for the 1979–2009 period, and variabilities on monthly and seasonality basis based on inter-annual averages during 31 years. The location scale considered nine locations providing information on; wave power roses, probabilities of occurrence and cumulative distribution functions of wave power in different power ranges, variation and trend of yearly average wave power, seasonal average wave power and its annual variations, and quantities of wave energy flux for different H_{m0} and T_{m-10} ranges. Results show that areas with the highest wave energy potential are located in the south-western part of the Black Sea. These areas are; Burgas–Rezovo with an average annual total energy of 43.9 MW h/m followed by Dolni Chiflik–Shkorpilovtsi with 37.3 MW h/m and Istanbul–Alacali with 36.1 MW h/m.

18/00499 Managing a renewable resource facing the risk of a regime shift in the ecological system

de Zeeuw, A. and He, X. *Resource and Energy Economics*, 2017, 48, 42–54.

Resource management has to take account of the possibility of regime shifts in the ecological system that provides the resource. Regime shifts are uncertain and lead to structural changes in the system dynamics, lowering the carrying capacity of the resource. Optimal management is driven by two considerations. First, it becomes precautionary if a higher stock of the renewable resource decreases the hazard of a regime shift. Second, it either becomes precautionary or more aggressive depending on the adjustments that are needed after the regime shift. This in turn depends on the elasticity of intertemporal substitution. In conclusion, facing the risk of a regime shift in the ecological system, optimal management is ambiguous but precautionary if the marginal hazard rate of the regime shift is sufficiently high.

18/00500 Microalgal biodiesel: a possible solution for India's energy security

Sharma, Y. C. and Singh, V. *Renewable and Sustainable Energy Reviews*, 2017, 67, 72–88.

Extreme accession in industrialization and urbanization is responsible for huge demand of fossil fuels which are depleting day by day. Hence, search for renewable energy resource has become a considerable challenge in recent years. Biodiesel has been recognized as an alternative fuel, non-toxic and biodegradable which is capable to replace the diesel fuel. In developing countries such as India, there is crisis of edible oil and the edible oil is imported to accomplish the demand. Based on the outline presented, it is observed that search for biodiesel sources should consider the feedstocks that do not require fertile land, do not compete with food crop, help in reduction of greenhouse gas emission as well as decrease the dependency on other nations. So, recently microalgae have emerged to be very auspicious feedstock for production of biodiesel. The present study deals with the systematic analyses of energy demand and greenhouse gas emission statistics of various nations as well as all the steps involved in overall process from algal strain selection to biodiesel production. With these challenges, the solutions in biodiesel production from microalgae were also shown. Though, biodiesel is economically viable, more inquisition as well as technological evolvement is required in this direction. To overcome these problems, policies based on usage of bio fuels derived by various nations which encourage biodiesel production, making them rival of conventional energy sources are needed.

18/00501 Optimal control of conventional hydropower plant retrofitted with a cascaded pumpback system powered by an on-site hydrokinetic system

Wamalwa, F. *et al*. *Energy Conversion and Management*, 2017, 132, 438–451.

This paper presents an optimal control strategy for a hydropower plant retrofitted with a hydrokinetic-powered cascaded pumpback system in dry season. Pumpback operation aims at recycling a part of the downstream discharge back to the main dam to maintain a high water level to optimize the energy value of the available water. The problem is formulated as a multi-objective optimization problem to simultaneously minimize the grid pumping energy demand, minimize the wear and tear associated with the switching frequency of the pumps, maximize the restoration of the volume of the dam through pumpback operation and maximize the use of on-site generated hydrokinetic power for pumping operation. The performance of the proposed cascaded model is compared with the classical single pump pumped storage model. Simulation results based on a practical case study shows that the cascaded pumpback model can reduce the pumping energy demand by up to 48.18% and increase the energy yield of the resultant system by up to 47.10% in dry season.

18/00502 Overview and comparative study of two control strategies used in 3-phase grid-connected inverters for renewable systems

Guerrero-Rodríguez, N. F. *et al*. *Renewable Energy Focus*, 2017, 19–20, 75–89.

In this paper, an overview of grid-connected renewable systems is presented, then two current-control strategies for three-phase grid-connected inverters are analysed: first, the well-known d–q control in the rotating synchronous reference frame (d–q axes) using proportional integral regulators is described, and secondly, the proportional resonant controller in the stationary reference frame ($\alpha\beta$ axes). In order to obtain a high efficiency of the system when the three-phase utility grid voltages are affected by harmonic pollution, a harmonic compensator (HC) structure is used with the Proportional Resonant controller, this due to the ease way to compensate harmonics when a proportional resonant control is utilized instead of a d–q control. Then both control strategies (d–q control and PR + HC) are analysed under harmonic pollution condition. For both strategies, a positive sequence detector plus a synchronous reference frame phase-look loop (PSD + dqPLL) is used as the synchronization algorithm. After the study, it was observed that the PR controller provides a greater facility for carrying out the harmonic compensation process helping to fulfil with the international standards. A model of a grid-connected photovoltaic system with a nominal power of 10 kW is used to evaluate and compare the performance of the current-control strategies. For this, a real-time digital simulator platform is used.

18/00503 Rotational speed control and electrical rated power of an oscillating-water-column wave energy converter

Falcão, A. F. O. *et al*. *Energy*, 2017, 120, 253–261.

The oscillating water column device equipped with an air turbine is regarded by many researchers and developers as the simplest and most reliable wave energy converter. It has been object of extensive development effort, including the deployment of prototypes into the sea. The maximization of the produced electrical energy involves the control of the rotational speed, which affects the hydrodynamic process of wave energy absorption, the turbine aerodynamics and the performance of the electrical equipment. In the paper, the overall performance of the plant is modelled as an integrated process, with the hydrodynamic modelling based on linear water wave theory. Special account is taken of the electrical efficiency dependence on the load factor and of the constraint introduced by electrical rated power as a power level that should not be exceeded. A case study was selected to investigate these issues: the existing bottom-standing plant on the shoreline of the island of Pico, in the Azores Archipelago. Results are presented for the control of the self-rectifying air turbine of biradial type and for the annually produced electrical energy as affected by turbine size and by electrical rated power.

18/00504 The importance of regret minimization in the choice for renewable energy programmes: evidence from a discrete choice experiment

Boeri, M. and Longo, A. *Energy Economics*, 2017, 63, 253–260.

This study provides a methodologically rigorous attempt to disentangle the impact of various factors – unobserved heterogeneity, information and environmental attitudes – on the inclination of individuals to exhibit either a utility maximization or a regret minimization behaviour in a discrete choice experiment for renewable energy programmes described by four attributes: greenhouse gas emissions, power outages, employment in the energy sector, and electricity bill. Here the authors explore the ability of different models – multinomial logit, random parameters logit, and hybrid latent class – and of different choice paradigms – utility maximization and regret minimization – in

explaining people's choices for renewable energy programmes. The 'pure' random regret random parameters logit model explains the choices of respondents better than other models, indicating that regret is an important choice paradigm, and that choices for renewable energy programmes are mostly driven by regret, rather than by rejoice. In particular, it was found that the respondents' choices are driven more by changes in greenhouse gas emissions than by reductions in power outages. Finally, it was found that changing the level of information to one attribute has no effect on choices, and that being a member of an environmental organization makes a respondent more likely to be associated with the utility maximization choice framework.

18/00505 The influence of channel geometry on tidal energy extraction in estuaries
Garcia-Oliva, M. *et al. Renewable Energy*, 2017, 101, 514–525.
A significant number of estuaries in the UK not only have a high tidal range but also exhibit strong tidal currents, where tidal farms could be used for energy extraction. The purpose of this study is to examine the influence that the geometry of the channel has on the impact of a tidal farm deployed in an estuary. A hydrodynamic model (Mike21) has been used to model several idealized estuaries with dimensions based on a group of locations suitable for tidal energy extraction in the UK. The maximum changes in low and high water levels with the tidal farm have been identified for each case and located within the estuary. The changes in the time for the low and high tides in a point inside the estuary have also been analysed. It is noted that the maximum changes in water levels due to the farm range from the order of mm to a few dm and the locations of these changes are strongly dependent on the geometry of each case. In addition, the effect is generally more noticeable in the increase of low water levels and the decrease of high water levels than vice-versa. This would be associated with the loss of intertidal areas and the reduction of flood risk levels. In terms of the changes in the time of low and high water levels, the effects of the farm are negligible in all cases.

18/00506 The unstudied barriers to widespread renewable energy deployment: fossil fuel price responses
Foster, E. *et al. Energy Policy*, 2017, 103, 258–264.
Renewable energy policy focuses on supporting the deployment of renewable power generators so as to reduce their costs through scale economies and technological learning. It is expected that, once cost parity with fossil fuel generation is achieved, a transition towards renewable power should continue without the need for further renewable energy subsidies. However, this reasoning implicitly assumes that the cost of fossil fuel power generation does not respond to the large-scale penetration of renewable power. In this paper the authors build a standard economic framework to test the validity of this assumption, particularly in the case of coal and gas fired power generation. It was found that it is likely that the cost of fossil fuel power generation will respond to the large scale penetration of renewables, thus making the renewable energy transition slower or more costly than anticipated. More analysis is needed in order to be able to quantify this effect, the occurrence of which should be considered in the renewable energy discourse.

18/00507 Using system dynamics modeling to evaluate the feasibility of ethanol supply chain in Brazil: the role of sugarcane yield, gasoline prices and sales tax rates
Demczuk, A. and Padula, A. D. *Biomass and Bioenergy*, 2017, 97, 186–211.
This paper explores how sugarcane yield, gasoline prices and sales tax rates affect the production and consumption of ethanol from sugarcane in Brazil. The system dynamics model of the sugarcane and ethanol production chain explores the impact of these variables to evaluate the feasibility of ethanol production. Using the VENSIM software different arrangements for sugarcane yield, gasoline prices and sales tax were simulated (horizon of 20 years). Brazil's federal government policy of gasoline price below the international price and the diversity of state sales tax rates produce distortions in the ethanol market and impose considerable constraints on the development of the ethanol industry. The simulations show that to ensure the feasibility of ethanol production, the pump price of regular gasoline would need to be US$1.95 per litre, which is far higher than the US$1.26 per litre currently charged. Public policies involving the liberalization of gasoline prices and the homogenization of the sales taxes on ethanol among the Brazilian states could reduce the distortions caused by these policies. These policies could contribute to reduce uncertainty in the ethanol sector and encourage technological and productive investments. Future research could add and evaluate the impacts of the environmental benefits of ethanol production and consumption (carbon trade market, payment for environmental services and bioelectricity production) and of sugarcane byproducts on its feasibility. The sensitivity analysis revealed the effectiveness of the model to support policies and managerial decision making process in the sugarcane ethanol sector.

18/00508 Wind and wave energy potential in southern Caspian Sea using uncertainty analysis
Amirinia, G. *et al. Energy*, 2017, 120, 332–345.
In this paper, uncertainties in determining the offshore wind and wave energies were considered to estimate the wind and wave energy potentials in the southern Caspian Sea. For this purpose, 11 years of ECMWF data in 210 points were collected in the study area for the analysis. First, a SWAN model for wave modelling was performed and then, the wave and wind energies were calculated using conventional analysis. Next, the uncertainties in air density, wind speed, wind speed distribution parameters, wind turbine power performance, peak wave period, significant wave height in each peak wave period, and wave energy converter were considered and a Monte Carlo simulation for 1000 years was conducted for uncertainty analysis. Results showed that uncertainty analysis results in almost 9% lower average wave power density and 7.3% less exploitable energy than conventional analysis. In addition, wind power density computed by uncertainty analysis was on average about 4% higher than that obtained with the conventional analysis; however, the exploitable wind energy resulting from uncertainty analysis was 3% lower than the values computed by conventional analysis.

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Fundamental science, analysis, instrumentation

18/00509 A hybrid methodology to predict gas permeability in nanoscale organic materials; a combination of fractal theory, kinetic theory of gases and Boltzmann transport equation
Behrang, A. and Kantzas, A. *Fuel*, 2017, 188, 239–245.
A theoretical methodology is developed to study the permeability of gas in organic tight porous media. In derivation of the equations, three main mechanisms of gas transport in organic porous media are taken into account. The modified fractal theory is used to explain viscous transport. Using the kinetic theory of gases, a similar formula derived in the authors' previous study is applied to study the slippage phenomenon and the Knudsen transport. The surface transport which shows the impact of the gas adsorption on the permeability is addressed by direct solution of the Boltzmann transport equation for a thin layer of adsorbed gas. The final equation is used to explore influences of the adsorbed layer thickness, grain surface specularity and pressure on the gas permeability. The presented approach is validated against available experimental data. An excellent agreement between the proposed theoretical model and experimental results are observed.

18/00510 Automating biostratigraphy in oil and gas exploration: introducing GeoDAISY
O'Neill, M. A. and Denos, M. *Journal of Petroleum Science and Engineering*, 2017, 149, 851–859.
Biostratigraphy is a key upstream activity. Drilling operations use biostratigraphic data derived from core samples extracted via boreholes (mud logging) in order to guide drilling processes and verify models of basin geology. Current manual data analysis relies on the existence of sufficient numbers of biostratigraphers to be available to fulfil industry needs. However, due to factors such as retirement, and that the number of people being trained in the requisite taxonomic skills has declined sharply over the last couple of decades; the available pool of expertise is dwindling. It is clear that if the high cost of drilling operations is taken into account, the current situation is untenable and in many ways represents a perfect storm. This pessimistic situation can be radically changed by augmenting human expertise using automated species identification tools based on artificial neural network technology. DAISY (digital automated identification system), a proven system of this sort, could revolutionize commercial biostratigraphy operations by enabling microfossil identification to be undertaken by technicians. This would yield immediate benefits for the industry as it would permit routine work to be performed quickly and accurately by less skilful, cheaper and therefore more available staff; freeing biostratigraphers to concentrate on non-routine, more complex tasks. The feasibility study presented here indicates that DAISY can consistently identify microfossils to species, with repeatable, high levels of accuracy.

Crucially, it can also act as a permanent repository for taxonomic knowledge, which is currently lost when experienced personnel retire. There might also be additional environmental and social benefits if this technology is widely adopted within the oil and gas sector: as DAISY technology is generic, it can easily be re-targeted to interpret seismic data or even to estimate the impact of upstream exploration activities on abutting ecosystems.

18/00511 Comparison of the mineral oil lifetime estimates obtained by differential scanning calorimetry, infrared spectroscopy, and dielectric dissipation factor measurements

Polansky, R. *et al. Thermochimica Acta*, 2017, 647, 86–93.

In this study, improved observables and new endpoint criteria were developed to assess the remaining useful life of mineral transformer oil using differential scanning calorimetry (DSC) and Fourier transform infrared spectroscopy (FT-IR). The tested oil was exposed to thermal ageing at temperatures of 110, 120 and 130 °C for times ranging from 100 to 2400 h. The intensity of the infrared spectral band of the low-temperature inhibitor and the temperature of the thermo-oxidative DSC peak were considered for evaluation. The obtained results were correlated with standardized dielectric dissipation factor ($\tan\delta$) measurements. The results indicated that the analysed observables changed continuously during the applied thermal ageing. The endpoint criteria were subsequently determined and Arrhenius diagrams were constructed. The results demonstrated that the determination of the actual state or the lifetime of the transformer oil via DSC or FT-IR may be beneficial in terms of reducing the measurement time, the influence of moisture on the measurement results and the oil volume required for the tests. Thus, DSC and FT-IR represent promising alternatives to dissipation factor measurements.

18/00512 Comprehensive analysis of initiation and propagation pressures in drilling induced fractures

Razavi, O. *et al. Journal of Petroleum Science and Engineering*, 2017, 149, 228–243.

A new experimental set-up was designed to carry out high-pressure borehole fracturing tests on cylindrical rock samples. The experimental set-up offers full control over borehole, confining, and pore pressures. Fracturing experiments were conducted on cylindrical Berea sandstone samples. Several injection cycles were carried out on each rock sample to measure the fracture initiation pressure (FIP) and the stable fracture propagation pressure (FPP) at various confining pressures. The measured FIP values were compared with Hubbert and Willis' model, and Rummel's model. The stable FPPs were measured using synthetic based mud (SBM) with and without lost circulation material (LCM), and compared with the large-scale fracturing experiments conducted at the Drilling Engineering Association (DEA) 13 investigation. This study shows that initiation of a drilling induced fracture (DIF) is best characterized by a fracture mechanics approach such as Rummel's model. The stable FPP value changes linearly with the minimum horizontal stress (S_{hmin}), and it is independent of the maximum horizontal stress (S_{hmax}) or the vertical stress (S_v). Also, the authors show that adding LCM to the drilling fluids significantly enhances the stable FPP.

18/00513 Determination of NMR T_2 cut-off for clay bound water in shales: a case study of Carynginia Formation, Perth Basin, Western Australia

Testamanti, M. N. and Rezaee, R. *Journal of Petroleum Science and Engineering*, 2017, 149, 497–503.

Low-field nuclear magnetic resonance (NMR) has proved to be a valuable tool for the petrophysical characterization of conventional reservoirs, but its effective application to unconventional reservoirs is still under research. Pore structure characterization of shales is particularly challenging due to the complexity of the pore network and the small size of pores. Using low-field NMR, the authors performed transverse relaxation (T_2) experiments on samples from the Perth Basin, Western Australia. The samples were initially saturated with KCl brine to obtain the total NMR porosity and T_2 distribution, then centrifuged and finally oven-dried at increasing temperatures. T_2 spectra were also acquired after centrifuging and heating the samples. The results indicate that most of the transverse relaxation occurs below 3 ms in saturated samples and that a conventional centrifuge cannot remove water from the smaller pores, making the commonly accepted clay bound water cut-off unsuitable for shales. Furthermore, the results from NMR experiments performed on the oven-dried shale samples suggest that the water content remains relatively constant after heating them above 65 °C. The calculated T_2 cut-off for clay bound water is between 0.22 and 0.26 ms for the samples studied. The methodology presented in this paper can be replicated in other formations to find a suitable T_2 value for clay bound water, which can be a good indication of potentially producible porosity and can also be used for permeability estimation.

18/00514 Development of nuclear forensic models using kernel regression

Jin, K. *et al. Progress in Nuclear Energy*, 2017, 94, 55–63.

The objective of nuclear forensics is to find out the origin or distribution process of illegal radioactive materials that are out of regulatory control by analysing some specific characteristics referred to as 'signatures'. One such radioactive material is nuclear spent fuel, which is likely to be intercepted in transit and abused. However, numerous samples of spent fuel cannot be obtained in Korea because analysing irradiated nuclear substances has been limited due to international regulations. Thus, in this paper, spent fuel sample data for nuclear forensics were generated using ORIGEN (ORNL Isotope Generation and Depletion code) based on operational histories of Korean nuclear power plants. This paper focuses on the development of a spent fuel inference model for nuclear forensics to estimate operational histories such as burn up, initial enrichment and cooling time for radioactive materials. The type of measurable nuclides and the accuracy of measured nuclides were assumed to be varied. Therefore, the regression model to estimate operational histories should be precise and robust. An inferential model based on kernel regression (IKR) that can provide estimates based only on data (without the assumptions required in physical models) has been developed in order to predict operational histories. On the other hand, the auto-associative model of kernel regression (AAKR) was used to eliminate some outliers in the input data to enhance the accuracy of the regression.

18/00515 Distributed temperature sensor testing in liquid sodium

Gerardi, C. *et al. Nuclear Engineering and Design*, 2017, 312, 59–65.

Rayleigh-backscatter-based distributed fibre optic sensors were immersed in sodium to obtain high-resolution liquid-sodium temperature measurements. Distributed temperature sensors (DTSs) functioned well up to 400 °C in a liquid sodium environment. The DTSs measured sodium column temperature and the temperature of a complex geometrical pattern that leveraged the flexibility of fibre optics. A single ∅ 360 µm OD sensor registered dozens of temperatures along a length of over one meter at 100 Hz. The capability to use a single DTS to simultaneously detect thermal interfaces (e.g. sodium level) and measure temperature was also demonstrated.

18/00516 Eigendecomposition model of resistance temperature detector with applications to S-CO_2 cycle sensing

Heifetz, A. and Vilim, R. *Nuclear Engineering and Design*, 2017, 311, 60–68.

Supercritical carbon dioxide (S-CO_2) is a promising thermodynamic cycle for advanced nuclear reactors and solar energy conversion applications. Dynamic control of the proposed recompression S-CO_2 cycle is accomplished with input from resistance temperature detector (RTD) measurements of the process fluid. One of the challenges in practical implementation of S-CO_2 cycle is high corrosion rate of component and sensor materials. In this paper, the authors develop a mathematical model of RTD sensing using eigendecomposition model of radial heat transfer in a layered long cylinder. It is shown that the value of RTD time constant primarily depends on the rate of heat transfer from the fluid to the outer wall of RTD. It is also demonstrated that for typical material properties, RTD time constant can be calculated as the sum of reciprocal eigenvalues of the heat transfer matrix. Using the computational model and a set of RTD and CO_2 fluid thermo-physical parameter values, the authors calculated the value of time constant of thermowell-mounted RTD sensor at the hot side of the precooler in the S-CO_2 cycle. The eigen decomposition model of RTD will be used in future studies to model sensor degradation and its impact on control of S-CO_2.

18/00517 Energy analytics in public buildings using interactive histograms

Blanco, I. D. *et al. Energy and Buildings*, 2017, 134, 94–104.

This paper proposes a visual analytics approach based on data cube methods to provide an insightful analysis of how energy is being used in a group of public buildings according to many different factors. The analysis is done by means of a web-based visual interface featuring 'live' coordinated views – histograms – that show the distribution of demand data, according to different attributes, under different scenarios defined by user-driven filters on these attributes. The authors use the crossfilter.js library to achieve real-time computation of data cube aggregations for constantly changing user-defined filters, resulting in a fluid visualization of demand parameters (active power, power factor, total harmonic distortion, etc.) aggregated according to many different factors or dimensions such as time (hour, day of week, month, etc.), building or environment (outside temperature).

18/00518 Environmental stress cracking in gamma-irradiated polycarbonate – a diffusion approach

de O. Silva, P. P. J. C. *et al. Radiation Physics and Chemistry*, 2017, 130, 123–132.

Polycarbonate (PC) is an engineering polymer which presents interesting properties. This material has been also used in medical devices, which is frequently exposed to gamma radiosterilization and to chemical agents. This may produce significant changes in polymer structure, leading to failure in service. The present work brings about a new approach on environmental stress cracking (ESC) processes elucidation in 100 kGy gamma-irradiated PC, by evaluating the diffusion process of methanol or 2-propanol in test specimens and determining the diffusion parameters on solvent-irradiated polymer systems. A comparison of diffusion parameters for both solvents indicated that methanol has a considerable ESC action on PC, with diffusion parameter of $7.5\times10^{-14}\pm1\%\,m^2\,s^{-1}$ for non-irradiated PC and $7.8\times10^{-14}\pm2.8\%\,m^2\,s^{-1}$ for PC irradiated at 100 kGy. In contrast, 2-propanol did not act as an ESC agent, as it did promote neither swelling nor cracks in the test specimens. These results were confirmed by visual analysis and optical microscopy. Unexpectedly, structural damages evidenced in tensile strength tests suggested that 2-propanol is as aggressive as methanol chemical for PC. Moreover, although some manufacturers indicate the use of 2-propanol as a cleaning product for PC artifacts, such use should be avoided in parts under mechanical stress.

18/00519 Forecasting method for global radiation time series without training phase: comparison with other well-known prediction methodologies

Voyant, C. *et al. Energy*, 2017, 120, 199–208.

Integration of unpredictable renewable energy sources into electrical networks intensifies the complexity of the grid management due to their intermittent and unforeseeable nature. Because of the strong increase of solar power generation the prediction of solar yields becomes more and more important. Electrical operators need an estimation of the future production. For nowcasting and short-term forecasting, the usual technics based on machine learning need large historical data sets of good quality during the training phase of predictors. However data are not always available and induce an advanced maintenance of meteorological stations, making the method inapplicable for poor instrumented or isolated sites. This paper proposes intuitive methodologies based on the Kalman filter use (also known as linear quadratic estimation), able to predict a global radiation time series without the need of historical data. The accuracy of these methods is compared to other classical data driven methods, for different horizons of prediction and time steps. The proposed approach shows interesting capabilities allowing to improve quasi-systematically the prediction. For one to 10 h horizons Kalman model performances are competitive in comparison to more sophisticated models such as ANN which require both consistent historical data sets and computational resources.

18/00520 Fracturing and calcite cementation controlling fluid flow in the shallow-water carbonates of the Jandaíra Formation, Brazil

de Graaf, S. *et al. Marine and Petroleum Geology*, 2017, 80, 382–393.

The shallow-marine carbonate rocks of the Jandaíra Formation have been subject to significant permeability variations through time due to various events of fracturing and calcite cementation. As a consequence, the Jandaíra Formation accommodated fluid flow only during specific moments in time. The authors reconstructed these episodes of fluid flow based on isotope characterizations and microscope characteristics of calcite veins and host rock cements. The Jandaíra Formation, which belongs to the post-rift sequence of the Potiguar Basin in northeast Brazil, was deposited from the Turonian onward until a marine regression exposed it in the Campanian. Due to the subaerial exposure, meteoric waters flushed out marine connate waters, leading to an event of early diagenesis and full cementation of the Jandaíra Formation. Fluid flow through the resulting impermeable carbonate formation appears to be closely related to fracturing. Fracturing in the Late Cretaceous induced a drastic increase in permeability, giving rise to extensive fluid circulation. Host rock dissolution associated to the circulating fluids led to calcite vein cementation within the fracture network, causing it to regain an impermeable and sealing character. In the research area, fluid flow occurred during early burial of the Jandaíra Formation at estimated depths of 400–900 m. This study documents the first application of fluid inclusion isotope analysis on vein precipitates, which allowed full isotopic characterization of the paleo-fluids responsible for calcite vein cementation. The fluid inclusion isotope data indicate that upwelling of groundwater from the underlying Açu sandstones provided the fluids to the fracture network. In Miocene times, renewed tectonic compression of a lower intensity created a secondary fracture network in the Jandaíra Formation. The density of this fracture network, however, was too low to induce a new episode of fluid circulation. As a result, this tectonic event is associated with the development of barren extensional fractures.

18/00521 Hydrothermal synthesis of single-crystal α-tristrontium phosphate particles

Ishida, A. *et al. Journal of the European Ceramic Society*, 2017, 37, (1), 351–357.

Anisotropic ceramic bodies can be fabricated by a reactive template grain growth method; however, template particles with suitable powder properties are required to create the ceramics with well controlled anisotropy. Therefore, well-isolated α-tristrontium phosphate (α-TSP) particles were synthesized with a hexagonal plate-like shape as template particles for anisotropic strontium apatite ceramics using α-strontium hydrogen phosphate (α-$SrHPO_4$) precursor particles. Three synthetic parameters were varied: (i) precursor particle size, (ii) stirring rate and (iii) hydrothermal temperature. Well-isolated hexagonal plate-like α-TSP single-crystal particles were successfully synthesized by hydrothermal treatment at 150 °C for 3 h at a stirring rate of 150 rpm using fine α-$SrHPO_4$ precursor particles. The developed plane of the hexagonal plate-like α-TSP particles was determined to be the {00*l*} plane, and the side planes were revealed to be not {*h*00} planes, but inclined {*h*0*l*} planes. The resulting α-TSP particles may provide a promising template for the development of anisotropic apatite-based ceramics.

18/00522 Ice-sheet dynamics through the Quaternary on the mid-Norwegian continental margin inferred from 3D seismic data

Montelli, A. *et al. Marine and Petroleum Geology*, 2017, 80, 228–242.

Reconstructing the evolution of ice sheets is critical to the understanding of the global environmental system, but most detailed palaeoglaciological reconstructions have hitherto focused on the very recent history of ice sheets. Here, the authors present a three-dimensional (3D) reconstruction of the changing nature of ice-sheet derived sedimentary architecture through the Quaternary Ice Age of almost 3 Ma. An extensive geophysical record documents a marine-terminating, calving Fennoscandian Ice Sheet (FIS) margin present periodically on the mid-Norwegian shelf since the beginning of the Quaternary. Spatial and temporal variability of the FIS is illustrated by the gradual development of fast-flowing ice streams and associated intensification of focused glacial erosion and sedimentation since that time. Buried subglacial landforms reveal a complex and dynamic ice sheet, with converging palaeo-ice streams and several flow-switching events that may reflect major changes in topography and basal thermal regime. Lack of major subglacial meltwater channels suggests a largely distributed drainage system beneath the marine-terminating part of the FIS. This palaeo-environmental examination of the FIS provides a useful framework for ice-sheet modelling and shows that fragmentary preservation of buried surfaces and variability of ice-sheet dynamics should be taken into account when reconstructing glacial history from spatially limited datasets.

18/00523 Improvement of mechanical and thermal properties of high energy electron beam irradiated HDPE/hydroxyapatite nano-composite

Mohammadi, M. *et al. Radiation Physics and Chemistry*, 2017, 130, 229–235.

In this research work, the nano-composites of high density polyethylene/hydroxyapatite samples were manufactured via two methods: In the first method, the granules of high density polyethylene and nano-structure hydroxyapatite were processed in an internal mixer to prepare the nano-composite samples with a different weight percentage of the reinforcement phase. As for the second one, high density polyethylene was prepared in nano-powder form in boiling xylene. During this procedure, the hydroxyapatite nano-powder was added with different weight percentages to the solvent to obtain the nano-composite. In both of the procedures, the used hydroxyapatite nano-powder was synthesized via hydrolysis methods. The samples were irradiated under 10 MeV electron beam in 70–200 kGy of doses. Mechanical, thermal and morphological properties of the samples were investigated and compared. The results demonstrate that the nano-composites prepared using nano-polyethylene, show better mechanical and thermal properties than the composites prepared from normal polyethylene granules, due to the better dispersion of nano-particles in the polymer matrix.

18/00524 Influence of alpha irradiation on pre and post solar exposed PM-355 polymeric nuclear track detector sheets

Alsalhi, M. S. *et al. Radiation Physics and Chemistry*, 2017, 130, 451–458.

The effect of alpha irradiation before and after solar exposed PM-355 polymeric SSNTDs films was investigated. The absorption spectra for both non-irradiated and irradiated samples at different solar exposure

time in different months showed a shift in the absorption edge towards lower wavelengths as the solar exposure time increases. This is probably ascribed to the presence of conjugate bonds. The fluorescence spectra indicated three distinguished peaks at approximately 330, 415 and 465 nm respectively. The first peak is attributed to the band gap while the other two peaks due to a probable formation of solid defects. The structure analysis using X-ray diffraction (XRD) proved the partial crystalline nature of the polymer with dominant amorphous phase. There was a slight increase in the XRD peak intensity for the sample irradiated by alpha particles indicating that the polymeric detector structure becomes more crystalline with a change in the crystallite size.

18/00525 Investigation of dual-energy X-ray photon counting using a cadmium telluride detector with dual-energy selection electronics

Sato, E. *et al. Radiation Physics and Chemistry*, 2017, 130, 385–390.

To obtain two kinds of tomograms at two different X-ray energy ranges simultaneously, the authors have developed a dual-energy X-ray photon counter with a cadmium telluride (CdTe) detector and two energy-selecting devices (ESDs). The ESD consists of two comparators and a microcomputer (MC). X-ray photons are detected using the CdTe detector, and the event pulses from a shaping amplifier are sent to two ESDs simultaneously to determine two energy ranges. X-ray photons in the two ranges are counted using the MCs, and the logical pulses from the MCs are input to frequency-to-voltage converters (FVCs). The outputs from the two FVCs are input to a personal computer through an analogue-to-digital converter to carry out dual-energy computed tomography. The tube voltage and current were 80 kV and 8.5 μA, respectively. Two tomograms were obtained simultaneously with two energy ranges. K-edge CT using iodine and gadolinium media was carried out utilizing two energy ranges of 33–45 and 50–65 keV, respectively. The maximum count rate was 6.8 kilo-counts per second with energies ranging from 10 to 80 keV, and the exposure time for tomography was 9.8 min.

18/00526 Magnetic-spring based energy harvesting from human motions: design, modeling and experiments

Wang, W. *et al. Energy Conversion and Management*, 2017, 132, 189–197.

A tuneable magnetic-spring based electromagnetic energy harvester is presented in this paper to harvest vibration energy from human motions. The harvester is modelled by Ansoft Maxwell software and the best way of magnetic stack is chosen according to the generated voltage from simulation. Dynamic model of the energy harvester is derived and corresponding theoretical and numerical analysis are performed to evaluate the performance of the proposed system. Experimental results under frequency-sweep excitation with different acceleration levels show that the harvester is promising to generate electricity for a broadband frequency range. In the experiments considering human motion, the impact between shoe and ground as well as the swing motion of leg are investigated by attaching the device to human lower-limb. Testing results under various motion speeds show that proper structural parameters such as equivalent mass and movement length can improve the performance of the harvester. Moreover, it is demonstrated that the swing motion of human lower-limb could enhance the performance of the proposed device, especially for higher motion speed.

18/00527 Material flow analysis (MFA) as a tool to improve ship recycling

Jain, K. P. *et al. Ocean Engineering*, 2017, 130, 674–683.

The shipowner's decision to select a recycling yard for dismantling and recycling an end-of-life ship is primarily influenced by the price offered for purchasing the ship. The recycling yards offering 'green' recycling services generally quote lower prices than other yards due to the higher cost of dismantling a ship by following international ship recycling regulations and health, safety and environmental (HSE) management systems. Such 'green' recycling yards must either lower their costs or increase their revenues to offer better prices to ship owners compared to the yards which have primitive or non-existent HSE standards. This article analyses multi-disciplinary scientific tools and techniques that can be used to make 'green' ship recycling economically attractive to ship owners without compromising HSE standards. Material flow analysis (MFA) has been found to be a suitable tool to analyse and plan the ship recycling process. This allows ship recycling yards to better manage waste and resources, thereby reducing costs. The material flow diagrams for a bulk carrier (case ship), showing the generic ship recycling process, are also developed and discussed. The analysis approach used in this article shows one way of introducing analytical tools into ship recycling planning and process assessment.

18/00528 Nonlinear technique and self-powered circuit for efficient piezoelectric energy harvesting under unloaded cases

Lallart, M. *Energy Conversion and Management*, 2017, 133, 444–457.

Vibration energy harvesting using piezoelectric materials has been intensively studied over the last few years, because of the wide availability of vibrational sources and the good integration and conversion abilities of piezoelectric materials. However, the power output of piezoelectric energy harvesters (PEH) is still limited due to the relatively low mechanical quality factor and coupling coefficient of the electromechanical structure. Recently, non-linear processes have been introduced to increase the energy extraction abilities of PEHs, showing impressive increase of the power output under monomodal excitation. However, their performance is limited when the structure is subjected to more complex signals or when considering the charge of a single capacitor (the latter operation reflecting well the typical use of self-powered systems). The purpose of this paper is to expose an enhancement of this technique, based on disabling the non-linear process if no harvesting event has been done previously. This therefore allows better energy conversion abilities under multimodal excitation as it allows a better control of the trade-off between the number of switching events and the voltage values at the switching instant, as well as increasing the harvested energy in monochromatic case, as the damping effect is limited. Finally, in order to dispose of realistic devices, a self-powered version of the enhanced technique is proposed and validated through simulation analysis and experimental implementation.

18/00529 Numerical study on the Welander oscillatory natural circulation problem using high-order numerical methods

Zou, L. *et al. Progress in Nuclear Energy*, 2017, 94, 162–172.

In this paper, high-order numerical methods are investigated in a system analysis-like code. The classical Welander oscillatory natural circulation problem, which resembles a simplified example for many types of natural circulation loops widely seen in nuclear reactor systems, was chosen to illustrate the applicability of such methods in system analysis codes, and to demonstrate the advantages of such methods over the low-order methods widely used in existing system analysis codes. As originally studied by Welander, the fluid motion in a differentially heated fluid loop can exhibit stable, weakly unstable, and strongly unstable modes. A theoretical stability map has also been originally derived from the stability analysis. Numerical results obtained in this paper show very good agreement with Welander's theoretical derivations. For stable cases, numerical results from both the high-order and low-order numerical methods agree well with the non-dimensional flow rate that were analytically derived. The high-order numerical methods give much less numerical errors compared to those using low-order numerical methods. For stability analysis, the high-order numerical methods perfectly predicted the stability map even with coarse mesh and large time step, while the low-order numerical methods failed to do so unless very fine mesh and time step are used. The result obtained in this paper is a strong evidence for the benefits of using high-order numerical methods over the low-order ones, when they are applied to simulate natural circulation phenomenon that has already gained increasing interests in many existing and advanced nuclear reactor designs.

18/00530 Paper-based origami flexible and foldable thermoelectric nanogenerator

Rojas, J. P. *et al. Nano Energy*, 2017, 31, 296–301.

Paper has been an essential material in daily life since ancient times. Its affordability, accessibility, adaptability, workability and its easiness of usage makes it an attractive structural material to develop many kinds of technologies such as flexible electronics, and energy storage and harvesting devices. Additionally, the scientific community has increased its interest on waste heat as an environmentally friendly energy source to support the increasing energy demand. Therefore, this paper describes two affordable and flexible thermoelectric nanogenerators (TEGs) developed on paper substrates by the usage of simple micromachining and microfabrication techniques. Moreover, they exhibit mechanical stability and adaptability (through folding and cutting techniques) for a diverse set of scenarios where vertical or horizontal schemes can be conveniently used depending on the final application. The first TEG device, implemented on standard paper, generated a power of 0.5 nW ($\Delta T = 50$ K). By changing the substrate to a tearless and extra-smooth polyester paper, the TEG performance was optimized achieving less internal resistance and a greater power of ~80 nW ($\Delta T = 75$ K), at the cost of more rigidity in the substrate. This power represented over three times higher power production than the standard paper-based TEG with same dimensions, number of thermoelectric pairs and temperature difference. Another interesting aspect of paper based TEG is due to its foldability, one can control the temperature difference by unfolding (larger separation between hot and cold ends) and folding (smaller separation). Finally, one of the

underlying objectives of this work is to spread the availability of essential technologies to the broad population by inclusion of everyday materials and simple processes.

18/00531 Procedure to assess the role of railway pantograph components in generating the aerodynamic uplift

Carnevale, M. *et al. Journal of Wind Engineering and Industrial Aerodynamics*, 2017, 160, 16–29.

The paper investigated the influence of aerodynamic forces on a railway pantograph's aerodynamic uplift, which significantly affect the mean value of the contact force exerted by the pantograph on the overhead line. The analysis was carried out by means of both wind tunnel tests on a full-scale pantograph and computational fluid dynamic (CFD) simulation in a wind tunnel scenario. The CFD model can be usefully adopted to evaluate numerical drag and lift forces acting on each single pantograph component, which is not easily performed experimentally, even in the wind tunnel. These forces can be used as the input of a procedure based on the virtual work principle, in order to evaluate the contribution of each different pantograph component to the total aerodynamic uplift. Due to the pantograph kinematics, the uplift is affected by both lift and drag forces acting on the single elements. Steady Reynolds-averaged Navier–Stokes (RANS) simulations appear sufficiently accurate to qualitatively reproduce the behaviour corresponding to different pantograph configurations, also giving satisfactory quantitative results, with computational effort compatible with their use at design stage. The most significant discrepancies were observed for pantograph components that are usually shielded, at least partially, in real line operation. The proposed methodology can, therefore, be usefully adopted as an aid for the pantograph design and for the preliminary assessment of the pantograph's aerodynamic behaviour, keeping on-line tests only for final verification and eventual fine-tuning. The obtained results do not account for the train roof boundary layer, which has the main effect of reducing the forces exerted on the lower parts of the pantograph due to the reduced velocity of the incoming flow. The presence of the train roof boundary layer should be considered (and simulated through the CFD calculation of the full train) for the evaluation of the actual aerodynamic uplift in the final operating condition.

18/00532 Quantitative risk assessment of submarine pipeline instability

Li, X. *et al. Journal of Loss Prevention in the Process Industries*, 2017, 45, 108–115.

Ensuring the on-bottom stability of the submarine pipeline is very important for safety concern during the operational stage of submarine pipeline. Due to the action of the external factors, e.g. strong current, wave and soil liquefaction, the submarine pipeline may have lateral displacement, vertical floatation or sinking. Although the submerged weight of submarine pipeline is designed to meet the requirement of on-bottom stability, the loss risk of pipeline on-bottom stability still exists due to the change of ocean environment or seabed. This paper presents a reliability-based assessment methodology for submarine pipeline instability. Firstly, a mechanical model of pipeline on-bottom state is built considering the hydrodynamic loads and pipe-soil interaction, which is the static forces equilibrium equations essentially, and a detailed analysis of loading condition of pipeline on seabed is also conducted. Then, based on the reliability theory, the limit state equations of pipeline instability are developed through converting the forces equilibrium equations. Because the parameters in limit state functions possess random uncertainty, such as wave and current loads, etc., the specific probability distributions are employed to present the random uncertainty of the parameters in limit state functions. The Monte Carlo method is then employed to solve the limit state equations for assessing the pipeline instability probability. The risk level of pipeline instability is judged using the risk ranking in DNV-RP-F107. The case study indicates that the proposed risk assessment methodology for pipeline instability possesses a good application performance. In essence, the assessment results could provide a powerful support for risk management or decision-making of submarine pipeline instability.

18/00533 Real-time monitoring of mechanical specific energy and bit wear using control engineering systems

Al-Sudani, J. A. *Journal of Petroleum Science and Engineering*, 2017, 149, 171–182.

Drilling of oil and gas wells utilize drilling mechanical energy to crush formation rocks through drill bits. Due to the friction with the formation rocks, the bit cutters suffer a continuous wear with the progress of the drilling causing reduction in rate of penetration. Real-time bit wear is a challenge in drilling as there is no absolute physical model. This paper presents new philosophy based on control engineering systems to simulate bit behaviour and estimate the transferred and wasted mechanical energy to predict drilling performance efficiency. Analytical model has been developed to predict drilling performance by analysing the real-time transferred drilling mechanical energy consumed by the drill bits, the model will assist in optimizing the hydraulic energy and take the proper time decision to pull the dulled bits. The model consists of a first order differential equation solved to predict the effect of drilling parameters on drill bit wear; while, the bit wear equation enters in a second order differential equation solved by Laplace transformation, and expressed as a transfer function representation which allows in analysing the drilling performance, and also expressed as real-time of bit displacement achieved by the input drilling energy. The poles of denominator of the transfer function have been analysed as a complex conjugate pairs; the location of the real part of the complex roots indicates the amount of real-time consumed mechanical energy by the drilling bits to destroy formation rocks. While, the location of imaginary roots indicates the amount of wasted mechanical energy due to bit wear. The effect of hydraulic energy on drilling performance has been simulated using closed loop transfer function, which allows for monitoring the wasted mechanical energy, and the wasted hours of bit life consumed in extra cutting due to insufficient hydraulic energy. The results show that the visual representation for poles location allows real-time monitoring for the performance of the transferred mechanical energy due to both bit dullness and to insufficient hydraulic energy explicitly. The results also show high decline rate in transferred mechanical energy always occurs within small values of bit dullness compared with that occurred in large values of bit dullness, which confirm the real field observations. The comparison with field examples proves the model reliability in predicting the drilling performance.

18/00534 Screening constant by unit nuclear charge calculations of resonance energies and widths of the 3p*n*s ^{1,3}P° and 3p*n*d ^{1}P° Rydberg series of Mg-like ($Z = 13$–26) ions

Khatri, I. *et al. Radiation Physics and Chemistry*, 2017, 130, 208–215.

Resonance energies and total natural width of the 3p*n*s ^{1}P° and 3p*n*d ^{1}P° Rydberg series of Mg-like ($Z = 13$–26) ions are reported. Resonance energies of the Mg-like Al^{+} belonging to the 3p*n*s $^{3}P^{\circ} \rightarrow 2p_6 3p_2 P^{0}_{1/2}$ and 3p*n*s $^{3}P^{\circ} \rightarrow 2p_6 3p_2 P^{0}_{3/2}$ transitions are also tabulated. The calculations are made in the framework of the screening constant by unit nuclear charge (SCUNC) formalism. Excellent agreements between experiments at ALS and *R*-matrix calculations are obtained for both 3p*n*s ^{1,3}P° and 3p*n*d ^{1}P° Rydberg series of the Mg-like Al^{+} ions. The present results for Mg-like Si^{2+}, S^{4+}, Cl^{5+} and Ar^{6+}, compared with the only existing *R*-matrix calculations indicate lack of accuracy in the Mg-like Si^{2+} data obtained from non-iterative formulation of the eigenchannel *R*-matrix method. New precise data for Mg-like P^{3+}, K^{7+}, Ca^{8+}, Sc^{9+}, Ti^{10+}, V^{11+}, Cr^{12+}, Mn^{13+} and Fe^{14+} ions are presented as useful guidelines for investigators focusing their challenge on the photoionization of Mg-like heavy charged ions in connection with their application in laboratory, astrophysics, and plasma physics.

18/00535 Synchrotron-based x-ray absorption spectroscopy for the electronic structure of $Li_xMn_{0.8}Fe_{0.2}PO_4$ mesocrystal in Li^{+} batteries

Wi, S. *et al. Nano Energy*, 2017, 31, 495–503.

The carbon-coated $LiMn_{0.8}Fe_{0.2}PO_4$ (LMFP) mesocrystal, composed of ~40-nm-sized nanocrystallites, was designed to be favourable for the fast charge transport kinetics. The carbon-coated LMFP mesocrystal exhibited good electrochemical properties (i.e. high specific capacity and superior rate capability), ensuring that the LMFP mesocrystal is a proper model system to study the reaction mechanism upon the battery cycling. In order to investigate the electronic-structure effects of each transition metal (Mn and Fe) on the electrochemical performance, the authors performed synchrotron-based soft and hard X-ray absorption spectroscopy (sXAS and XAS), and quantitatively analysed the changes of the transition-metal redox states in the carbon-coated LMFP electrodes during the electrochemical reaction. This comprehensive as well as complementary analyses using *ex situ* sXAS and *in situ* XAS can provide clear experimental evidence on the reaction mechanism of $LiMn_{0.8}Fe_{0.2}PO_4$ electrodes during battery operation.

18/00536 The performance of resistance, inductance, and capacitance handheld meters for determining moisture content of low-carbon fuels

Davis, J. *et al. Fuel*, 2017, 188, 254–266.

The moisture content (MC) of a fuel is generally determined through gravimetric analysis where a sample is dehydrated in an oven over a period of approximately 24 h; the MC is then calculated by dividing the difference between the initial and final mass, by the initial mass. Handheld moisture meters offer the benefit of near-instantaneous measurements and should provide accurate and dependable results. The performance of nine moisture meters applied to seven low-carbon fuels (LCFs) was determined. The nine meters employed three measurement technologies: electrical conductance/resistance, electrical capacitance and electromagnetic inductance. The seven LCF samples considered were: shredded switchgrass, two batches of shredded wood,

two batches of ragger tails and two batches of sanitary products. A moisture meter applicable for LCF should have a clear relationship between the actual MC and the measured MC, low variability, and be accurate within an absolute difference of 2%. Results indicated that none of the meters were suitable for use on LCF in general. It was not possible to identify a specific measurement technology that performed better for a certain LCF type from the results.

18/00537 Tracing the circulation of groundwater in volcanic systems using the $^{87}Sr/^{86}Sr$ ratio: application to Mt. Etna

Liotta, M. *et al. Journal of Volcanology and Geothermal Research*, 2017, 331, 102–107.

The $^{87}Sr/^{86}Sr$ ratio was investigated in groundwater circulating in the volcanic edifice of Mt. Etna in order to estimate the possible contribution of deep brines circulating in the sedimentary basement. Samples from 14 sites were collected and analysed for their chemical composition and Sr-isotope ratios. While the most common approach of coupling $^{87}Sr/^{86}Sr$ ratios with the concentration of dissolved Sr is not effective in distinguishing between the deep brine and seawater contributions, the authors suggest that the Sr/Cl ratio is a useful complementary parameter that needs to be considered when attempting to clearly identify the Sr sources. The obtained data indicate that the Sr-isotope signature of groundwater is determined by the volcanics hosting the aquifer. The volcanic isotopic signature is modified by very small amounts of brines ($< 1\%$), characterized by a high concentration of Sr and a $^{87}Sr/^{86}Sr$ ratio typical of sedimentary environments, but only at sites where the groundwater circulates almost in contact with the sedimentary basement. Conversely, the contribution of seawater is completely ruled out since this should produce a higher concentration of chloride. The proposed approach is potentially very effective for tracing the circulation of groundwater not only at Mt. Etna but also at volcanic edifices that overlie a bedrock with different $^{87}Sr/^{86}Sr$ ratios as well as at volcanic islands where freshwater overlies seawater.

18/00538 Ultrahigh current efficiency of light-emitting devices based on octadecylamine-graphene quantum dots

Kim, D. H. and Kim, T. W. *Nano Energy*, 2017, 32, 441–447.

Graphene quantum dots (GQDs) have currently emerged as excellent candidates for applications in GQD-based LEDs because of their potential applications in next-generation multifunctional systems. However, the numerous oxygenous functional groups and defects existing in the GQDs restrict their florescence quantum yield, resulting in a decrease in the brightness of light-emitting devices (LEDs) based on GQDs. Here, the authors report on solution-processed and highly-efficient LEDs that have been developed based on octadecylamine (ODA)-GQDs. In contrast with the GQDs, the number of oxygen components in the ODA-GQDs is lower due to nucleophilic substitution between the amine and the epoxy functional groups. The current and the external quantum efficiency of an LED with ODA-GQDs are 6.51 cd/A and 2.67%, respectively, this current efficiency of 6.51 cd/A being the highest among the efficiencies reported for LEDs based on GQDs. The efficiency enhancement in the LEDs with ODA-GQDs is attributed to significant improvements in the optical properties of the ODA-GQDs. The successful demonstration of this efficiency enhancement for LEDs based on ODA-GQDs indicates a potential for applications of GQD-based LEDs as next-generation real optical sources.

18/00539 Unsteady void measurements within debris beds using high speed X-ray tomography

Laurien, E. *et al. Nuclear Engineering and Design*, 2017, 312, 277–283.

Two-phase flow and boiling within debris beds representing a destroyed reactor core after a severe accident with core fragmentation can be simulated by using the porous media approach. In this approach, a local pressure drop and the heat transfer between the solid debris particles and the two-phase flow is modelled with the help flow-pattern maps, in which the boundaries between bubbly, slug, and annular flow are assumed. In order to support further understanding of these flows the authors have developed a very fast X-ray measurement device to visualize the 3D-void distribution within particle beds or porous media, which are otherwise unaccessible internally. The experimental setup uses a scanned electron beam directed in circles on a tungsten target to generate the X-rays. The particle bed, which has a diameter of 70 mm, is located between this target and a field of 256 X-ray detectors, which are arranged on a circle concentric to the target. The void distribution is reconstructed numerically from the attenuation of signals, which penetrates the particle bed and the two-phase flow inside. A 3D frame rate of up to 1000 Hz can be reached. The spatial resolution is such that bubbles with a diameter >1.7 mm can be detected. The authors have investigated two-phase flows air/water through beds of packed plastic spheres (with a diameter between 3 and 15 mm) as well as through plastic beds, which were manufactured using a '3D-plotter'. Flow patterns can be individually determined on the basis of empirical criteria. It is confirmed, that the transition between slug and annular flow depends on the air mass flux, but the particle diameter must be considered as an additional parameter.

18/00540 Video monitoring reveals pulsating vents and propagation path of fissure eruption during the March 2011 Pu'u 'Ō'ō eruption, Kilauea volcano

Witt, T. and Walter, T. R. *Journal of Volcanology and Geothermal Research*, 2017, 330, 43–55.

Lava fountains are a common eruptive feature of basaltic volcanoes. Many lava fountains result from fissure eruptions and are associated with the alignment of active vents and rising gas bubbles in the conduit. Visual reports suggest that lava fountain pulses may occur in chorus at adjacent vents. The mechanisms behind such a chorus of lava fountains and the underlying processes are, however, not fully understood. The March 2011 eruption at Pu'u 'Ō'ō (Kilauea volcano) was an exceptional fissure eruption that was well monitored and could be closely approached by field geologists. The fissure eruption occurred along groups of individual vents aligned above the feeding dyke. The authors investigated video data acquired during the early stages of the eruption to measure the height, width and velocity of the ejecta leaving eight vents. Using a Sobel edge-detection algorithm, the activity level of the lava fountains at the vents was determined, revealing a similarity in the eruption height and frequency. Based on this lava fountain time series, they estimated the direction and degree of correlation between the different vents. It was found that the height and velocity of the eruptions display a small but systematic shift in time along the vents, indicating a lateral migration of lava fountaining at a rate of ~11 m/s from west to east. This finding is in agreement with a propagation model of a pressure wave originating at the Kilauea volcano and propagating through the dyke at ~10 m/s from west to east. Based on this approach from videos only 30 s long, the authors were able to obtain indirect constraints on the physical dyke parameters, with important implications for lateral magma flow processes at depth. This work shows that the recording and analysis of video data provide important constraints on the mechanisms of lava fountain pulses. Even though the video sequence is short, it allows for the confirmation of the magma propagation direction and a first-order estimation of the dyke dimensions.

18/00541 Wind characteristics at bridge site in a deep-cutting gorge by wind tunnel test

Li, Y. *et al. Journal of Wind Engineering and Industrial Aerodynamics*, 2017, 160, 30–46.

To study the wind characteristics at bridge site in a deep-cutting gorge, a gigantic bridge site terrain model was made in a wind tunnel. The effects of different oncoming wind directions on the wind characteristics over the bridge site were investigated in the simulated atmospheric boundary layer. Results show that the perpendicular wind speed profiles along the bridge main beam can be generally divided into two parts. The shapes of the wind speed profiles at the two bridge towers are much closer to the power law and log law than those of the bridge main beam. The wind attack angle required for the wind resistant design of the bridge should be determined in the range of $-6°$ to $2°$, which obviously exceeds the range of $-3°$ to $3°$ that is usually considered in the homogeneous terrain. When the oncoming wind is from southwest, the wind power spectra at 1/4 span, mid-span and 3/4 span points match well with the spectra values by the Kaimal model. For two measurement points of the same distance, the decay factor of the coherence function varies along the bridge main beam as well as the bridge towers depending on their positions.

Fuel cell technology

18/00542 Effect of strontium [on] the phase structure of $Ba_{1-x}Sr_xCe_{0.65}Zr_{0.2}Y_{0.15}O_{3-\delta}$ ($0 \le x \le 0.25$) proton conductor by citrate–EDTA complexing sol–gel method

Sailaja, J. M. *et al. Journal of Asian Ceramic Societies*, 2017, 5, (1), 18–30.

Proton conducting oxides $Ba_{1-x}Sr_xCe_{0.65}Zr_{0.2}Y_{0.15}O_{3-\delta}$ ($0 \le x \le 0.25$) are prepared using the citrate–EDTA complexing sol–gel method. The effect of strontium and yttrium doping on the material properties is systematically investigated. The phase formation, thermal analysis, morphology, stability and conductivity measurements are performed on the sintered powders through TG–DTA, XRD, SEM, EDAX, FTIR, Raman and LCR measurements. The results indicated a single-phase orthorhombic system. Strontium incorporation helped in increasing the grain size up to 20% of strontium doping while reducing the lattice parameters and unit cell volume. The ionic conductivities of the $Ba_{1-x}Sr_xCe_{0.65}Zr_{0.2}Y_{0.15}O_{3-\delta}$ sintered oxides increased with increase in the concentration of Sr^{2+} along with the co-doping strategy

of trivalent Y^{3+} in the B site. Among the synthesized samples, $Ba_{0.8}Sr_{0.2}Ce_{0.65}Zr_{0.2}Y_{0.15}O_{3-\delta}$ pellet with orthorhombic structure showed highest conductivity with a value of 2.35×10^{-1} S/cm and 2.41×10^{-1} S/cm at 500 °C due to its smaller lattice volume, larger grain size and lower activation energy that led to excessive increase in conductivity. All pellets exhibited good chemical stability when exposed to air and H_2O atmospheres. These results indicate that this composition can be used as a potential electrolyte if synthesis conditions and temperature are well maintained.

18/00543 Engineering nanostructures of PGM-free oxygen-reduction catalysts using metal-organic frameworks

Zhang, H. *et al. Nano Energy*, 2017, 31, 331–350.

Oxygen reduction reaction (ORR) is one of the essential electrochemical reactions for the energy conversion and storage devices such as fuel cells and metal-air batteries. However, a large amount of Pt is required for catalysing the kinetically sluggish ORR at the air cathode, therefore greatly limiting their large scale implementation. Development of high-performance platinum group-metal (PGM)-free ORR catalysts has been a long-term goal for these clean energy technologies. However, current PGM-free catalysts are still significantly suffering from insufficient activity and limited durability especially in more challenging acidic media, such as proton exchange membrane (PEM) fuel cells. Recently, metal-organic frameworks (MOFs), constructed from bridging metal ions and ligands, have emerged as a new type of attractive precursors for the synthesis of PGM-free catalysts, which has led to encouraging performance improvement. Compared to other catalyst precursors, MOFs have well-defined crystal structure with readily tuneable chemistry and contain all required elements (e.g. carbon, nitrogen, and metal). Here, the authors provide an account of recent innovative PGM-free catalyst design and synthesis derived from the unique MOF precursors with special emphasis on engineering nanostructure and morphology of catalysts. The aim here was to provide new insights into the design and synthesis of advanced PGM-free catalysts with increased density of active sites and controlled bonding in 3D frame network. In addition, the possibility to use the well-defined MOF precursors for building up model systems to elucidate the structure-property correlations and the nature of active sites was also discussed.

18/00544 Flow field bipolar plates in a proton exchange membrane fuel cell: analysis & modeling

Kahraman, H. and Orhan, M. F. *Energy Conversion and Management*, 2017, 133, 363–384.

This study investigates flow fields and flow field plates (bipolar plates) in proton exchange membrane fuel cells. In this regard, the main design considerations and limitations for a flow field network have been examined, along with a comprehensive review of currently available flow field channel configurations. Also, the common materials and material properties used for flow field plates have been explored. Furthermore, a case study of step-by-step modelling for an optimum flow field design has been presented in-details. Finally, a parametric study has been conducted with respect to many design and performance parameters in a flow field plate.

18/00545 Heat integration of methanol steam reformer with a high-temperature polymeric electrolyte membrane fuel cell

Ribeirinha, P. *et al. Energy*, 2017, 120, 468–477.

A fuel cell is an exothermic device that wastes *ca*.50% of the input chemical energy while methanol steam-reforming (MSR) reaction is endothermic. The integration of a low temperature methanol steam-reforming cell (MSR-C) with a high temperature polymer electrolyte membrane fuel cell (HT-PEMFC) in a combined stack arrangement allows the thermal integration of both reactors. A novel bipolar plate of poly(p-phenylene sulfide) (PPS) featuring the fuel cell flow field in one side and the reformer flow field in the other was designed, built and assessed. For the first time are reported high current densities ($>0.5\,A\,cm^{-2}$) with the integrated system running at 453 K. The system was also ran for more than 100 h at 453 K, at $0.3\,A\,cm^{-2}$, with a methanol conversion of >90%. It was observed some degradation of the membrane electrode assembly (MEA) due to the continuous presence of methanol in the reformate stream. Electrochemical impedance spectroscopy (EIS) analyses revealed an overall increase of the resistances. The self-thermal sustainability of the combined device was only reached for $>0.75\,A\,cm^{-2}$ due to the poor thermal insulation of the combined reactor.

18/00546 Is microbial fuel cell technology ready? An economic answer towards industrial commercialization

Trapero, J. R. *et al. Applied Energy*, 2017, 185, 698–707.

Over the last decade, microbial fuel cells (MFCs) have experienced significant scientific and technological development, to the point of becoming close to commercialization. One key assessment that clearly establishes whether one technology can fully enter the market is the profitability demonstration. For this demonstration, classical evaluation criteria for investment decisions such as the net present value and the internal rate of return can be applied to a given proposal. This paper presents an economic assessment of a microbial fuel cell in a juice processing plant. Three different scenarios, optimistic, pessimistic and most likely scenarios based on the maximum power density of the cell on two basic MFC cases (cathodes with and without Pt, respectively), were studied and compared to the conventional activated sludge process. The results show that under most of the scenarios under consideration, including the pessimistic one, MFC is a more attractive option. Furthermore, a sensitivity analysis was performed with respect to the electrode area, and the annual growth rate of the electricity pricing has revealed that the electrode area parameter is the most influential, reducing the MFC profitability for larger electrode areas, whereas the higher the annual growth rates of the electricity price, the higher the MFC profits. In summary, the results of this study show that the implementation of MFC is a promising alternative to the use of classical aerated activated sludge, and it has potential economic benefits.

18/00547 Long term performance degradation analysis and optimization of anode supported solid oxide fuel cell stacks

Parhizkar, T. and Roshandel, R. *Energy Conversion and Management*, 2017, 133, 20–30.

The main objective of this work is minimizing the cost of electricity of solid oxide fuel cell stacks by decelerating degradation mechanisms rate in long term operation for stationary power generation applications. The degradation mechanisms in solid oxide fuel cells are caused by microstructural changes, reactions between lanthanum strontium manganite and electrolyte, poisoning by chromium, carburization on nickel particles, formation of nickel sulfide, nickel coarsening, nickel oxidation, loss of conductivity and crack formation in the electrolyte. The rate of degradation mechanisms depends on the cell operating conditions (cell voltage and fuel utilization). In this study, the degradation based optimization framework is developed which determines optimum operating conditions to achieve a minimum cost of electricity. To show the effectiveness of the developed framework, optimization results are compared with the case that system operates at its design point. Results illustrate optimum operating conditions decrease the cost of electricity by 7.12%. The performed study indicates that degradation based optimization is a beneficial concept for long term performance degradation analysis of energy conversion systems.

18/00548 Mathematical and experimental basis to model energy storage systems composed of electrolyzer, metal hydrides and fuel cells

Gonzatti, F. and Farret, F. A. *Energy Conversion and Management*, 2017, 132, 241–250.

With the increased integration of renewable energies in distribution networks comes the need for energy storage systems. Due to its characteristics, the use of hydrogen as an energy vector shows propitious features with this purpose. This study presents a type of storage energy system composed of an electrolyser, hydrogen accumulator and fuel cells. To model this system, it is necessary to establish a set of physicochemical equations for each component in order to integrate a large number of parameters and variables dependent on the model and operating conditions. This study describes a model for real storage power plants consisting of an alkaline electrolyser, a polymer electrolyte membrane fuel cell and a hydrogen accumulator in metal hydrides. A description of some practical tests on each component of the plant is included in order to compare them with the simulated results. All steps and parameters are discussed with the purpose of being used for other plants of similar characteristics.

18/00549 Nitrogen-enriched pseudographitic anode derived from silk cocoon with tunable flexibility for microbial fuel cells

Lu, M. *et al. Nano Energy*, 2017, 32, 382–388.

Microbial fuel cells (MFCs), promising for converting biomass energy into electricity, have attracted much research enthusiasm. However, high performance anode materials for MFC, particularly with tuneable flexibility for diverse cell configurations, are still limited. In this study, through a simple one-step carbonization of a versatile protein precursor, silk cocoon, both freestanding and flexible bioanode materials, with enriched nitrogen contents and hierarchical pores, can be easily fabricated. Importantly, the carbonized silk cocoon, as a freestanding MFC anode, and flexible carbon fibre, as a flexible MFC anode, exhibit high performance in electricity generation, yielding about 2.5-fold and 3.1-fold maximum gravimetric power density than that of MFCs with carbon cloth anode, respectively. The authors attribute the improved anode performance of these flexibility tuneable carbon materials to their good biocompatibility, reduced electron transfer resistance and high capacitance. This study will not only offer great opportunities for the fabrication of high-performance MFC

anode with varied designs and three-dimensional architectures, but also shed light on the future development of MFC and proper utilization of the abundant 'green' natural resources.

18/00550 Numerical simulation of the heat extraction in EGS with thermal-hydraulic-mechanical coupling method based on discrete fractures model

Sun, Z.-x. *et al. Energy*, 2017, 120, 20–33.

The enhanced geothermal system (EGS) creates an artificial geothermal reservoir by hydraulic fracturing which allows heat transmission through the fractures by the circulating fluids as they extract heat from hot dry rock (HDR). The technique involves complex thermal–hydraulic–mechanical (THM) coupling process. A numerical approach is presented in this paper to simulate and analyse the heat extraction process in EGS. The reservoir is regarded as fractured porous media consisting of rock matrix blocks and discrete fracture networks. Based on thermal non-equilibrium theory, the mathematical model of THM coupling process in fractured rock mass is used. The proposed model is validated by comparing it with several analytical solutions. An EGS case from Cooper Basin, Australia is simulated with 2D stochastically generated fracture model to study the characteristics of fluid flow, heat transfer and mechanical response in geothermal reservoir. The main parameters controlling the outlet temperature of EGS are also studied by sensitivity analysis. The results shows the significance of taking into account the THM coupling effects when investigating the efficiency and performance of EGS.

18/00551 Quantitative and qualitative investigation of the fuel utilization and introducing a novel calculation idea based on transfer phenomena in a polymer electrolyte membrane (PEM) fuel cell

Yousefkhani, M. B. *et al. Energy Conversion and Management*, 2017, 131, 90–98.

In this study, fuel utilization (U_F) of a polymer electrolyte membrane fuel cell (PEMFC) have been investigated within transfer phenomenon approach. Description of the U_F and fuel consumption measurement is the main factor to obtain the U_F. The differences between the experimental study and theoretical calculations results in the previous research articles reveal the available theoretical equations should be studied more based on the fundamental affairs of the U_F. Hence, there is a substantial issue that the U_F description satisfies the principles, and then it can be validated by the experimental results. The results of this study indicate that the U_F and power grew by 1.1% and 1%, respectively, based on one degree increased temperature. In addition, for every 1 kPa pressure increment, U_F improved considerably by 0.25% and 0.173% in the 40 and 80 °C, respectively. Furthermore, in the constant temperature, the power improved by 22% based on one atmospheric growth of the pressure. Results of this research show that the U_F has a differential nature, therefore differential equations will be employed to do an accurate theoretical calculation. Accordingly, it seems that the main defect of the theoretical calculation depends on Nernst equation that can be modified by a differential nature coefficient.

18/00552 Self-humidifying Pt-C/Pt-TiO_2 dual-catalyst electrode membrane assembly for proton-exchange membrane fuel cells

Yang, H. N. *et al. Energy*, 2017, 120, 12–19.

A high-performance Pt-C/Pt-TiO_2 dual-catalyst electrode was prepared and found to exhibit excellent water production and retention in self-humidifying proton-exchange membrane fuel cells. Different weight fractions of xPt-C/$(1-x)$Pt-TiO_2 dual-catalyst layer were applied to both anode and cathode with fixed total Pt loadings of 0.2 mg/cm^2 and 0.3 mg/cm^2. The dependence of cell performance on the Pt-TiO_2 content in dual-catalyst electrode was highly affected by the relative humidity (RH): When the RH was lower than 60%, the cell performance was significantly affected by the Pt-TiO_2 content. The ability to produce and retain water of the Pt-TiO_2 catalyst layer on the anode side was very important for the zero-RH cell performance. A visual cell experiment clearly revealed that water production at the anode was highly dependent on the Pt-TiO_2 content in the Pt-C/Pt-TiO_2 dual layer on the anode side. A half dual-layer experiment involving the Pt-TiO_2 on the cathode side alone strongly suggested that zero-RH operation is impracticable. The Pt-TiO_2 in the dual layer at the anode produces water consuming the H_2 and O_2 crossing the membrane from the cathode, resulting in excellent cell performance under zero RH. The Pt-C/Pt-TiO_2 ratio must be optimized in terms of the water-production and retention ability.

18/00553 Structure models and nano energy system design for proton exchange membrane fuel cells in electric energy vehicles

Li, Y. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 160–172.

Electric vehicles require fuel cells with a highly specific energy for the purpose of environmental protection and energy saving. However, proton exchange membrane vehicle fuel cells (PEMFC) face problems in terms of energy conversion efficiency, power density, costs and lifespan. This paper reviews key technical issues regarding the application of vehicle PEMFC especially the integration of nano-electro-catalytic energy system with high-performance electrolyte membranes. It also discusses the relation between vehicle PEMFC membrane structures and electrode performance revealing the nanostructured system model and the membrane electrode interface characterization. Manipulation of vehicle PEMFC electrode structure and quantitative characterization of the nanoscale catalyst interface are summarized aiming at improving Pt utilization efficiency, ionic conductivity and nano membrane electrode performance.

18/00554 Techno-economic analysis of polymer electrolyte membrane fuel cell system configurations

Mukhtar, B. *et al. Renewable Energy Focus*, 2017, 19–20, 38–48.

The major constraints restricting widespread commercialization of fuel cell systems are both technical and economical. Many researchers have designed polymer electrolyte membrane (PEM) fuel cell system configurations, which are different in terms of energy utilization and cost. Therefore, it is imperative to determine the best system configuration in order to produce efficient and economically viable PEM fuel cell systems. This paper reports an exergy and economic analyses conducted on five different PEM fuel cell system configurations with a view to assess their performance. Thermolib – a tool box for MATLAB/Simulink designed for modelling and simulation of energy systems was used to model and simulate the operation of each of the systems (5 kW stack power, 40 cells and 0.25 m^2 active membrane area) and data obtained was used for the exergy analysis. It was found that largest exergy loss occurred in the fuel cell stack (over 90%). The overall exergy and energy efficiencies of the studied systems were between 24.23% to 30.18% and 47.77% to 59.48%, respectively. A hybrid PEM fuel cell system configuration was proposed and analysed. It was found to have an overall exergy and energy efficiencies of 31.95% and 62.97%, respectively. The return-on-investment evaluated for each of the five studied PEM fuel cell system configurations as well as the proposed system configuration were 1–27% while the payback periods were 3–13 years. The proposed system configuration was found to have the best performance in terms of energy utilization and had the lowest cost per kilowatt net power.

18/00555 Thermal conditions and heat transfer characteristics of high-temperature solid oxide fuel cells investigated by three-dimensional numerical simulations

Lee, S. *et al. Energy*, 2017, 120, 293–305.

Elucidating internal thermal conditions of high-temperature solid oxide fuel cell (SOFC) stacks is essential for obtaining a substantial thermal efficiency and reliability for long-term operations prior to their commercialization. To examine simultaneous heat transfer and its generation and their effect on the local thermodynamic state, a high-fidelity physical model that resolves spatially the three-dimensional structure of planar, anode-supported SOFC stacks is used in this study. Results show that thermal conduction through metallic interconnects plays a key role in transferring the heat produced by joule heating and electrochemical reactions and thus determining the internal thermal conditions. The heat generated from the electrolyte and thin reactive electrode layers is transferred to the interconnect predominantly by gaseous convection and conduction through materials in the anode and cathode, respectively. The interconnect subsequently transports this heat conductively towards gas inlets and/or surrounding repeating units, influencing temperature increments, its profile and hot spot formation. Its effect on the internal thermal conditions was further examined by a parametric study with respect to the thermal property and geometry of the interconnect which determine its thermal resistance. They indeed affect significantly heat generation and its transfer within the cell, through its boundaries, between repeating units and to incoming gases.

18/00556 Thermodynamic performance assessment of an integrated geothermal powered supercritical regenerative organic Rankine cycle and parabolic trough solar collectors

Cakici, D. M. *et al. Energy*, 2017, 120, 306–319.

In this study, the thermodynamic performance of an integrated geothermal powered supercritical regenerative organic Rankine cycle (ORC) and parabolic trough solar collectors (PTSC) is assessed. A thermal model based on the principles of thermodynamics (mass, energy, and exergy balances) and heat transfer is first developed for the components of this integrated system. This model gives the performance assessment parameters of the system such as the electrical and exergetic efficiencies, total exergy destruction and loss, productivity lack, fuel depletion ratio, and improvement potential rate. To validate this model, the data of an existing geothermal power plant based on a supercritical ORC and literature data for the PTSC are used. After

validation, parametric studies are conducted to assess the effect of some of the important design and operating parameters on the performance of the system. As a result of these studies, it is found that the integration of ORC and PTSC systems increases the net power output but decreases the electrical and exergetic efficiencies of the integrated system. It is also shown that R134a is the most suitable working fluid type for this system; and the PTSCs and air cooled condenser are the main sources of the exergy destructions.

18/00557 Ti/(Ti,Cr)N/CrN multilayer coated 316L stainless steel by arc ion plating as bipolar plates for proton exchange membrane fuel cells
Wang, S. *et al. Journal of Energy Chemistry*, 2017, 26, (1), 168–174.
Arc ion plating (AIP) is applied to form Ti/(Ti,Cr)N/CrN multilayer coating on the surface of 316L stainless steel (SS316L) as bipolar plates for proton exchange membrane fuel cells (PEMFCs). The characterizations of the coating are analysed by scanning electron microscopy (SEM) and X-ray diffraction. Interfacial contact resistance between the coated sample and carbon paper is 4.9 $m\Omega\,cm^2$ under 150 N/cm^2, which is much lower than that of the SS316L substrate. Potentiodynamic and potentiostatic tests are performed in the simulated PEMFC working conditions to investigate the corrosion behaviours of the coated sample. Superior anticorrosion performance is observed for the coated sample, whose corrosion current density is 0.12 $\mu A/cm^2$. Surface morphology results after corrosion tests indicate that the substrate is well protected by the multilayer coating. Performances of the single cell with the multilayer coated SS316L bipolar plate are improved significantly compared with that of the cell with the uncoated SS316L bipolar plate, presenting a great potential for PEMFC application.

18/00558 Towards a better Sn: efficient electrocatalytic reduction of CO_2 to formate by Sn/SnS_2 derived from SnS_2 nanosheets
Li, F. *et al. Nano Energy*, 2017, 31, 270–277.
Electrocatalytic reduction of CO_2 into liquid fuels using electricity from renewable sources has been attracting considerable interest because of the present energy and environmental crisis. However, current electrocatalysts for this reaction generally suffer from either high cost for noble metal based catalysts or low energetic efficiency and poor product selectivity for other transition metal or carbon based materials. In this paper, the authors report a catalyst based on two-dimensional SnS_2 nanosheets supported on reduced graphene oxide (SnS_2/rGO) synthesized by a 'one-pot' hydrothermal reaction for electrocatalytic reduction of CO_2 into formate with high activity, selectivity and durability. The catalyst is capable of producing formate at an overpotential as low as 0.23 V and reaches a maximum faradaic efficiency of 84.5% and the current density of 13.9 $mA\,cm^{-2}$ at an overpotential of 0.68 V in aqueous bicarbonate medium. Microscopic, spectroscopic and electrochemical characterizations reveal that the electrocatalytic activity towards CO_2 reduction arises from the presence of reduced metallic tin formed from SnS_2 under cathodic electrolysis conditions; the enhanced performance is attributed to the residual SnS_2. This sulfide-derived metal catalyst with enhanced performance may open a perspective on a new promising class of materials for electrocatalytic reduction of CO_2.

18/00559 Transport phenomena in alkaline direct ethanol fuel cells for sustainable energy production
An, L. and Zhao, T. S. *Journal of Power Sources*, 2017, 341, 199–211.
Alkaline direct ethanol fuel cells (DEFC), which convert the chemical energy stored in ethanol directly into electricity, are one of the most promising energy-conversion devices for portable, mobile and stationary power applications, primarily because this type of fuel cell runs on a carbon-neutral, sustainable fuel and the electrocatalytic and membrane materials that constitute the cell are relatively inexpensive. As a result, the alkaline DEFC technology has undergone a rapid progress over the last decade. This paper provides a comprehensive review of transport phenomena of various species in this fuel cell system. The past investigations into how the design and structural parameters of membrane electrode assemblies and the operating parameters affect the fuel cell performance are discussed. In addition, future perspectives and challenges with regard to transport phenomena in this fuel cell system are also highlighted.

15 ENVIRONMENT

Pollution, health protection, applications

18/00560 A Bayesian modeling approach of human interactions with shading and electric lighting systems in private offices
Sadeghi, S. A. *et al. Energy and Buildings*, 2017, 134, 185–201.
This paper presents a hierarchical Bayesian approach to model human interactions with motorized roller shades and dimmable electric lights. At the top level of hierarchy, Bayesian multivariate binary-choice logit models predict the probability of shade raising/lowering actions as well as the actions to increase the level of electric light. At the bottom level, Bayesian regression models with built-in physical constraints estimate the magnitude of actions, and hence the corresponding operating states of shading and electric lighting systems. The models are based on a dataset from a field study conducted in private offices designed to facilitate a large number of participants and to collect data on environmental parameters as well as individual characteristics and human attributes governing human-shading and – electric lighting interactions. In this study, models were developed only for arrival periods due to the low frequency of actions during intermediate time intervals with continuous occupation. The modelling framework demonstrates the advantages of the Bayesian approach that captures the epistemic uncertainty in the model parameters, which is important when dealing with small-sized datasets, a ubiquitous issue in human data collection in actual buildings; it also enables the incorporation of prior beliefs about the systems; and offers a systematic way to select amongst different models using the Bayes factor and the evidence for each model. The findings reveal that besides environmental variables, human attributes are significant predictors of human interactions, and improve the predictive performance when incorporated as features in shading action models.

18/00561 An empirical classification-based framework for the safety criticality assessment of energy production systems, in presence of inconsistent data
Wang, T.-R. *et al. Reliability Engineering & System Safety*, 2017, 157, 139–151.
The technical problem addressed in the present paper is the assessment of the safety criticality of energy production systems. An empirical classification model is developed, based on the majority rule sorting method, to evaluate the class of criticality of the plant/system of interest, with respect to safety. The model is built on the basis of a (limited-size) set of data representing the characteristics of a number of plants and their corresponding criticality classes, as assigned by experts. The construction of the classification model may raise two issues. First, the classification examples provided by the experts may contain contradictions: a validation of the consistency of the considered dataset is, thus, required. Second, uncertainty affects the process: a quantitative assessment of the performance of the classification model is, thus, in order, in terms of accuracy and confidence in the class assignments. In this paper, two approaches are proposed to tackle the first issue: the inconsistencies in the data examples are 'resolved' by deleting or relaxing, respectively, some constraints in the model construction process. Three methods are proposed to address the second issue: (i) a model retrieval-based approach, (ii) the bootstrap method and (iii) the cross-validation technique. Numerical analyses are presented with reference to an artificial case study regarding the classification of nuclear power plants.

18/00562 Au@Cu_7S_4 yolk@shell nanocrystal-decorated TiO_2 nanowires as an all-day-active photocatalyst for environmental purification
Chiu, Y.-H. and Hsu, Y.-J. *Nano Energy*, 2017, 31, 286–295.
A vital issue that degrades the entirety of photocatalysis on TiO_2 is the requisite of light illumination for performing redox reactions. The ability to maintain the catalytic activity in dark environment has been the ultimate goal for the widespread deployment of TiO_2 photocatalysts. Here, for the first time the authors reported the demonstration of an all-day-active photocatalyst model by employing Au@Cu_7S_4 yolk@shell nanocrystal-decorated TiO_2 nanowires. The samples were obtained by depositing a Cu_2O layer on the Au surface of Au particle-decorated TiO_2 nanowires, followed by the sulfidation treatment on Cu_2O layer to grow hollow Cu_7S_4 shell. By coupling the pronounced charge separation and distinctive peroxidase mimic properties from the constituents, the TiO_2-Au@Cu_7S_4 nanowires were capable of performing efficient methyl orange degradation under light

illumination, yet still persisted noticeable activity of decomposing methyl orange after light irradiation was switched off. This study has embodied a conceptually valuable design of permanently working photocatalysts, which may serve as a versatile platform for the widely distributed environmental and energy applications such as pollutant destruction and organic transformation.

18/00563 Biorefinery site selection using a stepwise biogeophysical and social analysis approach

Martinkus, N. *et al. Biomass and Bioenergy*, 2017, 97, 139–148.

A key factor in the production of economically viable and environmentally sustainable biofuels is biorefinery site selection. Facility location analysis has traditionally been driven by access to feedstock, proximity to customers, and local incentives. While economic constraints will always be major factors in site selection, incorporating social metrics may further reduce the cost of constructing a biorefinery. A community's disposition toward a biorefinery project may significantly impact implementation success: grassroots support can lower implementation costs while opposition may increase the costs of permitting blockages and other scale-up delays. The proposed biorefinery siting tool improves upon previous research by incorporating site-specific biogeophysical measures and more complete and comprehensive social measures of community innovation and capacity for collective action. A refined biogeophysical analysis assesses pulp mills for their potential as repurposed biorefineries. The social asset components of site selection are greatly improved by enhancing and disaggregating key metrics through the use of multiple indicators of community collective action capacity and propensity for change. The refined measures are integrated into a biorefinery site-selection tool. Pulp mills that rank highly in both the biogeophysical and social asset measures may be considered more suitable candidates for repurpose into a biorefinery. This enriched methodology has been applied to biorefinery siting decisions in the US Pacific Northwest region; however, it is suitable for applications to infrastructure development projects in any region of the USA.

18/00564 Climate change and adaptive decision making: responses from North Carolina coastal officials

Bulla, B. R. *et al. Ocean & Coastal Management*, 2017, 135, 25–33.

While climate change is a global phenomenon, adaptive action starts at the local level. Understanding how local decision makers make sense of climate change and the decision to adapt or not is imperative for advancing action on climate change. This article advances the scholarship on local decision making about adaptive action through a study of North Carolina (NC) coastal communities that face an assortment of threats from climate change. During March and April 2014, 283 officials were surveyed across the 20 NC coastal counties to explore their willingness to take adaptive action (WTAA). The study utilized five risk scenarios to probe officials' knowledge about climate change, whether they perceived climate change as a threat to their community, and their political ideology. Findings indicated an officials' professed knowledge of climate change was not associated with WTAA. Officials who perceived climate change as a threat to their community were largely more WTAA. However, when the perceived threat was identified as uncertain, no significant relationships were identified. Findings for political ideology and WTAA indicated no significant differences under a low level of risk, yet under an average level of risk and an uncertain level of risk moderates were more WTAA than conservatives. Under higher than average and very high levels of risk moderates were more WTAA than both liberals and conservatives.

18/00565 Does technology diffusion help to reduce emission intensity? Evidence from organized manufacturing and agriculture in India

Majumdar, D. and Kar, S. *Resource and Energy Economics*, 2017, 48, 30–41.

This paper measures the 'emission intensity' of the 15 organized manufacturing and agricultural sectors in India. The primary objective and contribution in this paper are in obtaining a direct relation between technological adoption (greater capitalization) and emission intensity at the industry level over a period of 14 years between 1996 and 2009. The authors used the environmentally extended input–output model to calculate the direct, upstream and total emission intensity generated through the entire supply chain of production and consumption. From the fixed effects panel regression results, it was noted that technological adoption helps to reduce emission intensity across industries, although, beyond a critical level it raises the intensity. Importantly, when better technologies are adopted for production of export goods as against non-traded goods, emission falls in a significant way.

18/00566 Explaining citizens' perceptions of international climate-policy relevance

Schleich, J. and Faure, C. *Energy Policy*, 2017, 103, 62–71.

This paper empirically analyses the antecedents of citizens' perceptions of the relevance of international climate policy. Its use of representative surveys in the USA, China and Germany controls for different environmental attitudes and socio-economic factors between countries. The findings of the micro-econometric analysis suggest that the perceived relevance of international climate policy is positively affected by its perceived effectiveness, approval of the key topics discussed at international climate conferences, and environmental attitudes, but is not affected by perceived procedural justice. A higher level of perceived trust in international climate policy was positively related to perceived relevance in the USA and in China, but not in Germany. Citizens who felt that they were well informed and that their position was represented at climate summits were more likely to perceive international climate policy as relevant in China in particular. Generally, the results show only weak evidence of socio-demographic effects.

18/00567 Formation of gas discharging from Taketomi submarine hot spring off Ishigaki Island in the southern Ryukyu Islands, Japan

Toki, T. *et al. Journal of Volcanology and Geothermal Research*, 2017, 330, 24–35.

Taketomi submarine hot spring lies off Ishigaki Island in the southern Ryukyu Islands and vents hot spring waters at temperatures up to ~50 °C from the seafloor at a depth of 20 m. The authors investigated the chemical and isotopic composition of gases discharging from Taketomi hot spring. The gases were composed mainly of methane, with secondary nitrogen at higher than atmospheric concentration. Carbon and hydrogen isotope data suggest that the methane in the discharging gases was derived mainly from thermal decomposition of organic matter. Helium isotopes were enriched in ^{3}He relative to the atmosphere, suggesting a supply of mantle-derived helium to the discharging gases. The mantle-derived gases transfer the deep-originated thermal energy to the hot spring and thermogenesis of organic matter. The hydrocarbons in the venting gas could be sourced from sedimentary rocks of the Yaeyama or Shimajiri Groups, or Yaeyama metamorphic rocks, and added to the ascending gases as they pass through those source rocks on their way to the surface. Because the Pleistocene rocks of the Ryukyu Group beneath the hot spring have been altered by the spring activity, the Taketomi hot spring began venting after the Pleistocene.

18/00568 Interaction effects of building technology and resident behavior on energy consumption in residential buildings

Zhao, D. *et al. Energy and Buildings*, 2017, 134, 223–233.

Buildings account for a significant portion of energy consumption and carbon emissions around the world and increasingly scholars and practitioners are re-thinking strategies that mitigate use. This paper reports an empirical study aimed at identifying the relationship between building technology and resident behaviour and the joint effects on energy consumption in residential buildings. Unlike previous work that isolated effects of technology or behaviour on energy consumption, this study investigates their interactions. The researchers collected technical and behavioural data from more than 300 residential units and performed data analysis using energy simulation and multivariate regression techniques. Results identify the interaction effects between building technology and resident behaviour and provide quantifiable evidence supporting the hypothesis that 'building technology and resident behaviours interact with each other and ultimately affect home energy consumption'. Findings indicate four important resident behaviours that directly correlate to energy consumption and two that indirectly correlate to energy consumption. The research also indicates that only 42% of technological advances directly contribute to home energy efficiency, suggesting that the achievable impact on energy savings depends on both technical advances and behavioural plasticity.

18/00569 'Lock-in' effect of emission standard and its impact on the choice of market based instruments

Haoqi, Q. *et al. Energy Economics*, 2017, 63, 41–50.

A country's existing emission standard policy will lead to a 'lock in' effect. When the country plans to adopt new market-based instruments to control greenhouse gas emissions, it must consider this effect as it chooses among instruments to avoid larger efficiency loss. In this paper, the authors find that the 'lock in' effect will cause a kink point to occur on the marginal abatement cost (MAC) curve. This change of shape for the MAC curve is a reminder to be cautious in choosing market-based instruments when applying Weitzman's rule. The authors also introduce this concept into a dynamic multi-regional computable general equilibrium (CGE) model for China and simulate MAC curves for all regions. After applying Weitzman's rule, a timeline for introducing price instruments under different marginal benefit (MB) curve scenarios was proposed.

18/00570 Optimal sizing of residential PV-systems from a household and social cost perspective: a case study in Austria

Hartner, M. *et al. Solar Energy*, 2017, 141, 49–58.

This study analysed optimal sizing of grid connected rooftop photovoltaic systems from a household's perspective. The authors estimate the profit maximizing size for more than 800 households in Austria for various electricity tariffs and subsidy schemes considering economies of scale related to the investment costs of photovoltaic systems in the size range of 1–20 kW of installed capacity. Size dependent investment costs are estimated from data on photovoltaic systems installed in Austria from 2008 to 2013. They then take a social cost perspective and relate the results to the total investment costs to install a certain amount of capacity in residential areas. It was found that in the presence of economies of scale substantial cost inefficiencies can occur resulting from incentives to install relatively small systems. Depending on the compensation scheme the simulated optimal system size can be as low as 2 kW resulting in high costs per capacity. Subsidy design and tariff regulations can be adopted to incentivize larger photovoltaic systems in the residential sector which would reduce the costs of achieving a certain level of distributed PV generation. It is estimated that for a minimum system size of 5 kW total investment costs for subsidised residential photovoltaic systems in Austria from 2008 to 2013 could have been 2.2% lower for the same amount of installed capacity. It is further argued that the strict focus on onsite use of electricity from photovoltaic systems in the residential area is not necessarily desirable from a social cost perspective because it can lead to small and therefore more expensive photovoltaic systems.

18/00571 Post-rift sequence architecture and stratigraphy in the Oligo–Miocene Sardinia Rift (Western Mediterranean Sea)

Reuter, M. *et al. Marine and Petroleum Geology*, 2017, 79, 44–63.

Rift basins provide important sedimentary archives to reconstruct past tectonic and climatic conditions. Understanding their sedimentary history is, however, largely hampered by the competing influence of tectonic versus climatic forcing. The aim of this study is to comprehend the effects of local to regional tectonic and global climatic/eustatic changes on shallow marine depositional systems in the Sardinia Rift (western Mediterranean Sea). For this purpose the stratigraphic and depositional relations of a mixed siliciclastic-carbonate ramp at the Porto Torres Basin margin were studied along extensive proximal to distal transects. Three depositional sequences (DS1 to DS3) of late Burdigalian to early Serravallian age have been identified, which are separated by erosional unconformities. Each contains a lower transgressive part and an upper regressive part. The former includes shoreface sandstone (DS2) or coral reef (DS3) deposits on the proximal ramp and channelized sheet sandstone (DS1) or basinal mudstone (DS2, DS3) deposits on the distal ramp, typically recording an upsection trend of sediment starvation. The latter is represented by basinward-prograding coralline red algal carbonate wedges due to enhanced shallow water carbonate production rates. In the long term, the depositional evolution from DS1 to DS3 reveals basin margin progradation associated with decreasing siliciclastic supply. Integrated calcareous nannoplankton-foraminiferal-pectinid biostratigraphy links the depositional sequences to third-order sea-level cycles and allows to correlate the erosional unconformities at the top of DS1 and DS2 with the Bur 5/Lan 1 and Lan 2/Ser 1 sequence boundaries. The improved sequence stratigraphic framework enables better regional and global correlations. This shows that rhodalgal carbonate slopes started prograding in the western branch of the Sardinia Rift during the late Burdigalian because (1) of a worldwide bloom of rhodalgal facies, and (2) decreasing tectonic activity at the transition from the syn-rift to the post-rift stage caused a continuous reduction of the siliciclastic sediment input.

18/00572 Sustainable perspectives on energy consumption, EMRF, environment, health and accident risks associated with the use of mobile phones

Velmurugan, M. S. *Renewable and Sustainable Energy Reviews*, 2017, 67, 192–206.

Mobile phones have grown rapidly using today's wireless technology thereby providing a new dimension to simplify daily routine jobs by users. Mobile phone's applications have a great impact on the way of faster and more effective to convey information. In contrast, mobile phones could harm its users. This paper explored detrimental effects of mobile phones on energy consumption, electromagnetic radiofrequency radiation, environment, health and accidents. The effect of mobile phone's energy consumption can be considered during energy spend for its production and use. The electromagnetic radiofrequency radiation (EMRF) may cause adverse health effects on human. The raw materials which are used to manufacture for mobile phones may cause the severe environmental impacts due to their levels of toxicity. The health hazards are correlated with high-toxic substances released from the mobile phones and its addiction through a prolonged use. Mobile phone usage while driving can cause road traffic collisions and motor vehicle crashes. Furthermore, sustainable perspectives have been suggested as a way to overcoming these detrimental effects of mobile phones.

18/00573 Synthesis and performance evaluation of a novel biodegradable dispersant for offshore cementing

Wang, C. *et al. Journal of Natural Gas Science and Engineering*, 2017, 38, 582–589.

The authors developed a novel biodegradable oil-well dispersant, gelatin grafted acetone formaldehyde sulfonates (GAFS). This dispersant was prepared based on the chemical modification of naturally biodegradable products: gelatin. GAFS was synthesized through aldehyde ketone addition, hydroxyl condensation and Mannich amine methylation reaction. Functional groups and molecular structure of GAFS were characterized by Fourier transform infrared spectroscopy and nuclear magnetic resonance. Laboratory tests were conducted to determine the biodegradation rate, rheological properties, thickening time, compressive strength and dispersing property of GAFS in Class-G cement slurry. It was found that GAFS exhibits no retarding by-effect on oil well cement and can be considered biodegradable based on the biodegradation test results. The measured adsorption capacity and zeta potential of GAFS in Class-G well cement slurry show that: GAFS can be adsorbed greatly onto the surface of cement particles, resulting in strong electrostatic repulsion between cement particles and consequently generating an excellent dispersion performance.

18/00574 The substitution of wind power for coal-fired power to realize China's CO_2 emissions reduction targets in 2020 and 2030

Zhao, X. *et al. Energy*, 2017, 120, 164–178.

China's power industry contributes around 40% CO_2 emissions to the national total. The substitution of wind power for coal-fired power is crucial to the realization of CO_2 emission reduction target in China. By deploying the life cycle assessment (LCA) method, this paper identifies that the carbon footprints of a representative coal-fired plant and a wind farm in China are 810.35 and 12.51 g/kWh, respectively. Built on these results, the substitution capacities of wind power for coal-fired power to realize the CO_2 emission reduction target in 2020 and 2030 are discussed. It is concluded that China's wind power needs to develop faster than the goal set in the 12th Five-Year Renewable Energy Development Plan for achieving the target of 45% emission reduction in 2020. Moreover, the feasibility of the substitution of wind power for coal-fired power is analysed. It is argued that whilst China has great potential to realize such substitution given its rich wind resources, the full realization of the substitution requires some radical reforms in the power sector in the country.

18/00575 The trigger matters: the decision-making process for heating systems in the residential building sector

Hecher, M. *et al. Energy Policy*, 2017, 102, 288–306.

As heat demand of buildings accounts for a significant amount of final energy use and related carbon emissions, it is important to gain insights into the homeowners' decision-making processes and to identify factors determining the choice of heating systems. In this study, data was collected in an online survey carried out in 2015, from private homeowners of existing and newly built single and double-family houses in Austria who had invested in a new heating system within the last 10 years ($N = 484$). In contrast to previous studies, this study specifically investigates the triggers behind homeowner decisions to invest in a new heating system (e.g. problem, opportunity, or new building situation). Results of binary logistic regression analysis show that subsidies for heating system tab investments and infrastructural adjustments reveal to be most effective for homeowners in problem situations to foster alternative heating systems. For homeowners in opportunity situations (e.g. building refurbishment), in addition operational convenience appears to be important. For new buildings, the main barriers for alternative heating system adoption were found in the positive perception of fuel supply security and feasibility of fossil systems. Thus, the use of trigger-specific policy measures is proposed to foster alternative heating systems in the residential building sector.

18/00576 Ultrasensitive cellular fluorocarbon piezoelectret pressure sensor for self-powered human physiological monitoring

Wang, B. *et al. Nano Energy*, 2017, 32, 42–49.

Flexible and wearable pressure sensors are of essential importance in developing artificial electronic skin (e-skin) for areas such as healthcare monitoring and clinical diagnosis. Here, the authors report an ultrasensitive cellular fluorocarbon piezoelectret pressure sensor (FPS) via a three-step hot-pressing method. By constructing micron-sized voids in the inner cell, and combination with outstanding charge storage ability of the fluorocarbon electrets, tremendous piezoelectric activity can be obtained. The flexible FPS showed advantages of remarkable sensitivity (7380 pC N^{-1}) in the subtle-pressure regime

(<1 kPa), fast response time (50 ms), very low limit of detection (5 Pa) as well as high stability (30,000 cycles). In addition, the flexible and self-powered FPS owns the capability for detecting human motions such as wrist stretching, cheek motion from open–bite–open, eyes blinking and chest respiration, respectively. It can be also used for monitoring human physiological signals such as radial artery pulse wave. By virtue of easy processability in large scale, light weight, and low cost, the FPS is especially suitable for mass production and flexible electronics, indicating their promising applications in artificial intelligence and mobile healthcare monitoring systems.

CO_2, NO_x, SO_2 and particulate emissions

18/00577 Characteristics of CO_2 hydrate formation/dissociation in H_2O + THF aqueous solution and estimation of CO_2 emission reduction by district cooling application

Kim, S. *et al. Energy*, 2017, 120, 362–373.

CO_2 conversion by gas hydrate is considered one of most practical technologies in the fields of carbon capture, utilization and storage (CCUS). In this study, the effects of hydrate formation pressure and concentration of tetrahydrofuran (THF) on the CO_2 + THF hydrate formation and dissociation performance are investigated, and the reduction of CO_2 emission by applying the CO_2 + THF hydrate for district cooling system is also evaluated. The CO_2 capture ratio tends to increase with increasing the hydrate formation pressure and THF concentration. It is found that the CO_2 regeneration rate increases with decreasing the formation pressure and the increasing rate decreases with time. It is concluded that the optimum conditions for the CO_2 + THF hydrate formation and dissociation are 1.5 MPa, THF 1.5 mol% to use hydrate slurry as the working fluid for district cooling application. Also, the dissociation enthalpy of CO_2 + THF hydrate was measured by using the high pressure micro-differential scanning calorimeter. The cycle simulation of hydrate cooling system is conducted, and the COP is estimated as 11.55. Finally, it is estimated that 20,684 tons of CO_2 emission could be reduced per year if the CO_2 + THF hydrate technology is applied to the district cooling system of 51,600 RT.

18/00578 Fuel consumption and CO_2 emissions from passenger cars in Europe – laboratory versus real-world emissions

Fontaras, G. *et al. Progress in Energy and Combustion Science*, 2017, 60, 97–131.

Official laboratory-measured monitoring data indicate a progressive decline in the average fuel consumption and CO_2 emissions of the European passenger car fleet. There is increasing evidence to suggest that officially reported CO_2 values do not reflect the actual performance of the vehicles on the road. A reported difference of 30–40% between official values and real-world estimates was found which has been continuously increasing. This paper reviews the influence of different factors that affect fuel consumption and CO_2 emissions on the road and in the laboratory. Factors such as driving behaviour, vehicle configuration and traffic conditions are reconfirmed as highly influential. Neglected factors (e.g. side winds, rain, road grade), which may have significant contributions in fuel consumption in real world driving are identified. The margins of the present certification procedure contribute between 10 and 20% in the gap between the reported values and reality. The latter was estimated to be of the order of 40%, or 47.5 gCO_2/km for 2015 average fleet emissions, but could range up to 60% or down to 19% depending on prevailing traffic conditions. The introduction of a new test protocol is expected to bridge about half of the present divergence between laboratory and real world. Finally, substantial literature was found on the topic; however, the lack of common test procedures, analysis tools, and coordinated activity across different countries point out the need for additional research in order to support targeted actions for real world CO_2 reduction. Quality checks of the CO_2 certification procedure, and the reported values, combined with in-use consumption monitoring could be used to assess the gap on a continuous basis.

18/00579 Minimizing energy consumption in refrigerated vehicles through alternative external wall

Adekomaya, O. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 89–93.

Transporting fresh foods and raw agricultural produce have been widely acknowledged as a critical aspect of food chain. Raw fresh food must be conveyed at a low temperature conditions to preserve quality and prolong the shelf life of transported food. This paper takes an insight look at food transport system and proffers a sustainable ways of reducing energy consumption in diesel engine driven vapour compression system. Many studies have reported that 15% of world total energy is used in food preservation while some authors have predicted additional 2% annual increment of energy demand to sustain food chain. In the course of this study, the authors pragmatically identified sources of energy demand in food transport and maintained that the best approach to minimize energy consumption in refrigerated vehicles is to find a light weight and low thermal conductivity material as the external wall of refrigerated vehicles. This research is of high interest in view of continuous rise in earth temperature occasioned by emission of carbon monoxide from fossil fuel. The authors further showed that the usage of aluminium sheet as external wall of refrigerated vehicles reduces the longevity of insulation which increases heat infiltration into the cooling chamber thereby aggravating energy demand.

18/00580 Phase equilibrium of CCS mixtures: equation of state modeling and Monte Carlo simulation

Xu, X. *et al. The Journal of Supercritical Fluids*, 2017, 119, 169–202.

To understand the role played by the impurities (such as N_2, Ar, H_2, CO, SO_2, O_2 and NO) during the processes of carbon dioxide capture and storage (CCS), it is essential to know the thermodynamic properties of the CO_2-impurities mixtures under the conditions of CO_2 capture, transport and storage. Considering the variety of composition of these gas mixtures, it is necessary to have at one's disposal suitable models to predict their thermodynamic properties. In this work, two thermodynamic models: the *E*-PPR78 (Enhanced Predictive Peng-Robinson, 1978) and the PC-SAFT (Perturbed-Chain Statistical Associating Fluid Theory) models, are applied for describing the phase equilibria properties of 77 binary CCS mixtures containing CO_2, gas impurities (SO_2, O_2 and NO), water and hydrocarbons. This research results indicate that both models are able to accurately predict the phase behaviour of binary CCS mixtures. It was however necessary to adjust the binary interaction parameters ($k_{ij,\text{PC-SAFT}}$) within the PC-SAFT model to improve the prediction accuracy. Compared to the PC-SAFT model with one temperature-independent binary interaction parameter, the *E*-PPR78 model normally shows better prediction accuracy for the investigated systems. In addition, to extend the experimental database which was built for the evaluations of Equation-of-State (EoS) modelling, the Monte Carlo (MC) simulation method is employed in this work to generate phase-equilibrium data of a few CCS mixtures deemed as insufficiently described by experimental measurements reported in the open literature.

18/00581 Re-estimating CO_2 emission factors for gasoline passenger cars adding driving behaviour characteristics – a case study of Beijing

Li, Y. *et al. Energy Policy*, 2017, 102, 353–361.

The transportation sector is one of the largest sources of energy consumption and CO_2 emissions. The most important and difficult step in estimating transportation CO_2 emissions is to accurately estimate vehicle CO_2 emission factors (EFs). Most of the conventional methods draw less attention to driving behaviours. Based on a questionnaire survey, this study built a three-layer modified progressive regression model which included driving behaviours, and integrated vehicle and traffic characteristics. The results showed that for gasoline passenger cars with seven seats or fewer in Beijing, EFs were significantly affected by engine displacement (D), vehicle age (G), producing country, the proportion of annual total mileage on national, provincial and municipal roads except freeways (P), waiting mode for a red light when the waiting time is more than 1 min (W), and whether the windows were open while driving faster than 60 km/h (E). The influence order is: D (0.908) > W(−0.199) > E(0.080) > P(0.063) > producing country (−0.048, 0.042, <0.001 for J, A and C, respectively). More than 60 s flame out waiting time and closing windows while velocity more than 60 km/h can reduce 23.38 g CO_2/km and 8.93 g CO_2/km, respectively. The method to estimate vehicle EFs in this study can be used in other countries, and can provide scientific support for policymakers to implement traffic-control and CO_2-reduction measures.

18/00582 Retrieval and intercomparison of volcanic SO_2 injection height and eruption time from satellite maps and ground-based observations

Pardini, F. *et al. Journal of Volcanology and Geothermal Research*, 2017, 331, 79–91.

Syneruptive gas flux time series can, in principle, be retrieved from satellite maps of SO_2 collected during and immediately after volcanic eruptions, and used to gain insights into the volcanic processes which drive the volcanic activity. Determination of the age and height of volcanic plumes are key prerequisites for such calculations. However, these parameters are challenging to constrain using satellite-based techniques. Here, imagery was used from OMI and GOME-2 satellite sensors and a novel numerical procedure based on back-trajectory analysis to calculate plume height as a function of position at the satellite measurement time together with plume injection height and time at a volcanic vent location. The authors applied this new

procedure to three Etna eruptions (12 August 2011, 18 March 2012 and 12 April 2013) and compared their results with independent satellite and ground-based estimations. They also compared their injection height time-series with measurements of volcanic tremor, which reflects the eruption intensity, showing a good match between these two datasets. The results are a milestone in progressing towards reliable determination of gas flux data from satellite-derived SO_2 maps during volcanic eruptions, which would be of great value for operational management of explosive eruptions.

18/00583 Solar photo-thermochemical reactor design for carbon dioxide processing

Bhatta, S. *et al. Solar Energy*, 2017, 142, 253–266.

The direct use of solar energy for chemical processing, such as the synthesis of solar fuels, is an appealing alternative to mitigate environmental emissions while fulfilling the global demand for fuels. The design and evaluation of a direct solar receiver-reactor designed for gas-phase chemical synthesis is presented. The design rationale aims to promote concurrent gas-phase thermochemical and photochemical reactions below 1000 °C. The stainless-steel reactor chamber is designed to act as a light trapping cavity to increase photon absorption and to induce long gas residence times through a porous catalytic monolith. The experimentally determined radiative flux distribution map from a high-flux solar simulator is used for the dimensioning of the reactor's optical aperture. Metal (Cu) catalytic monoliths, designed to have relatively large specific surface and adequate light transmission, are evaluated to determine their light attenuation characteristics and resistance to fluid flow. The designed reactor is evaluated with the direct decomposition of carbon dioxide (CO_2). A computational fluid dynamics (CFD) model is used to analyse the reactor design and complement experimental evaluations. The model describes the gas flow throughout the chamber together with radiation transport and heterogeneous chemistry across the porous catalytic monolith. Experimental results are used for validation of the CFD model and to calibrate kinetic parameters of the heterogeneous chemical kinetics model. The findings indicate sub-optimal light transmission through the catalytic monolith given the rapid conversion of incident radiation into heat, and prompts to the need for co-optimization of the catalytic monolith's porous structure for light transmission and heterogeneous reactivity. The experimental results show a marked increase in CO_2 reduction efficiency with increasing radiation flux but the CO_2 decomposition with Cu catalyst is negligible at the tested temperatures. The reactor design methodology and evaluation can assist the devising of equipment and processes for the synergistic use of high-temperature photo- and thermo-catalysts to potentially allow CO_2 conversion at lower temperatures than exclusively solar thermochemical processes.

18/00584 Study on the ratio of pore-pressure/stress changes during fluid injection and its implications for CO_2 geologic storage

Kim, S. and Hosseini, S. A. *Journal of Petroleum Science and Engineering*, 2017, 149, 138–150.

The success of fluid injection into geological formations, which is the main operation during both carbon dioxide (CO_2) geologic storage and wastewater injection, is contingent on the geomechanical integrity of the site. A key task that allows us to evaluate the risk of geomechanical failure is the precise prediction of pore-pressure buildup and subsequent change in the state of stresses during and after the fluid injection. Contrary to traditional approaches, where total stresses are assumed to remain constant, recent studies have ascertained that total stresses in fact change in every direction as fluid extraction/injection disturbs the pore-pressure field and causes deformations. In this study, the authors conduct an in-depth investigation of the ratio of change in total stress to that in pore-pressure, $\Delta\Sigma/\Delta P$, which has been denoted in the literature as the pore-pressure/stress coupling. They used a numerical simulation method that couples single-phase fluid flow in porous media with poroelasticity to explore the spatiotemporal evolution of the $\Delta\Sigma/\Delta P$ ratio for various conditions. These numerical experiments allowed the examination of how different material properties and structural geometries would influence the evolution of $\Delta\Sigma/\Delta P$ in both vertical and horizontal directions. These ratios of pore-pressure/stress changes exhibited different spatiotemporal evolutions depending on key factors that include the hydraulic boundary condition, Biot's coefficient, Poisson's ratio, and the hydraulic diffusivity of both the injection zone and caprock. On the basis of observations, first-hand guidelines are suggested for analytically determining the ratio of pore-pressure/stress changes, $\Delta\Sigma/\Delta P$. Finally, the authors used examples and case studies to illustrate how the $\Delta\Sigma/\Delta P$ ratio can be incorporated into an analytic calculation for determining a maximum sustainable pressure limit.

18/00585 The lithium storage performance of electrolytic-carbon from CO_2

Tang, J. *et al. Journal of Power Sources*, 2017, 341, 419–426.

Sustainable and affordable energy resources are urgently demanded to mitigate environmental issues. Herein, carbon materials, prepared by electrochemical reduction of greenhouse gas, CO_2, in Li–Na–K carbonate molten salts (electrolytic-carbon), are tested as negative electrode materials for Li-ion batteries. Owing to the small particle size and suitable surface area, the electrolytic-carbon exhibits a high reversible capacity of 798 mAh g^{-1} (more than two times of graphites' theoretical capacity) at 50 mA g^{-1} and 266 mAh g^{-1} with a stable cyclability over 500 cycles at a current density up to 500 mA g^{-1}, as well as remarkable rate performance. Furthermore, a comprehensively study was conducted to investigate the effects of electrolysis temperature and cell voltage on the electrochemical performance of the electrolytic-carbon. These results demonstrate a promising strategy to develop renewable high-performance carbon negative electrode materials for Li-ion batteries by molten salt capture and electrochemical reduction of CO_2.

Hydrocarbon emissions

18/00586 Assessment of exposure to polycyclic aromatic hydrocarbons in preschool children: levels and impact of preschool indoor air on excretion of main urinary monohydroxyl metabolites

Oliveira, M. *et al. Journal of Hazardous Materials*, 2017, 322, 357–369.

This study aimed to assess the exposure of preschool children to polycyclic aromatic hydrocarbons (PAHs) by environmental monitoring (18 compounds in air) and biomonitoring [six urinary biomarkers of exposure (OH-PAHs)]. The impact of preschool indoor air on excretion of urinary monohydroxyl metabolites was also evaluated. Gaseous and particulate-bound PAHs were simultaneously collected indoors and outdoors in two Portuguese preschools. PAHs and OH-PAHs were quantified by high-performance liquid chromatography with fluorescence and photodiode array detection. Total air (gaseous + total suspended particles) levels of PAHs (ΣPAHs) were higher indoors than outdoors. Gaseous phase (composed by ≥98% of two- or three-ring compounds) and particulate-bound PAHs (90–99% of five or six rings) accounted for 93–95% and 5–7% of ΣPAHs in indoor air, respectively. Total (including probable/possible) carcinogenic PAHs represented 26–45% of ΣPAHs; naphthalene and dibenz[a,h]anthracene were the strongest contributors. A similar distribution profile was observed between airborne PAHs and urinary OH-PAHs. Urinary 1-hydroxynaphthalene + 1-hydroxyacenaphthene represented more than 78% of ΣOH-PAHs, being followed by 2-hydroxyfluorene, 1-hydroxypyrene, and 1-hydroxyphenanthrene. 3-Hydroxybenzo[a]pyrene (PAH biomarker of carcinogenicity) was not detected. Results suggest that children had preschool indoor air as their major exposure source of naphthalene and acenaphthene, while no conclusion was reached regarding fluorene, phenanthrene and pyrene.

18/00587 Ionic liquid technology to recover volatile organic compounds (VOCs)

Salar-García, M. J. *et al. Journal of Hazardous Materials*, 2017, 321, 484–499.

Volatile organic compounds (VOCs) comprise a wide variety of carbon-based materials which are volatile at relatively low temperatures. Most of VOCs pose a hazard to both human health and the environment. For this reason, in the last years, big efforts have been made to develop efficient techniques for the recovery of VOCs produced from industry. The use of ionic liquids (ILs) is among the most promising separation technologies in this field. This article offers a critical overview on the use of ionic liquids for the separation of VOCs both in bulk and in immobilized form. It covers the most relevant works within this field and provides a global outlook on the limitations and future prospects of this technology. The extraction processes of VOCs by using different IL-based assemblies are described in detail and compared with conventional methods This review also underlines the advantages and limitations posed by ionic liquids according to the nature of the cation and the anions present in their structure and the stability of the membrane configurations in which ILs are used as liquid phase.

18/00588 Iron bound to soil organic matter catalyzes H_2O_2 to oxidize crude oil in soil

Xu, J. *et al. Journal of Hazardous Materials*, 2017, 322, 516–524.

Under the action of hydrogen peroxide, soil organic matter (SOM) can transform dissolved iron (Fe^{2+}) into the solid phase. Solid iron is bound to SOM (Fe-SOM), and two components are included: iron oxides bound to SOM (Fe-SOM oxides) and organic iron bound to SOM (organic Fe-SOM). In oil-contaminated soil samples with Fe-SOM, total petroleum hydrocarbon (TPH) was degraded by 67%;

however, in oil-contaminated soil samples without Fe-SOM, the degradation of TPH was only 6%. In oil-contaminated soil samples with Fe-SOM, 73–86% of the primary alkanes (C_{14}-C_{22} composed 67.5% of TPH) were removed, whereas only 45–65% of the C_{12}-C_{13} and C_{22}-C_{30} alkanes were removed. The 11 types of alkanes (C_{12}-C_{13} and C_{22}-C_{30}) accounted for only 32.5% of TPH. Obviously, the degradation of TPH by Fe-SOM is independent of its hydrophobicity in the solid phase. The results also demonstrated that at a higher content of Fe-SOM, more hydroxyl radical (·OH) was produced in the solid phase and more TPH was degraded. A large number of ·OH are generated near iron–SOM–oil interface.

Life cycle analysis

18/00589 A life-cycle comparison of the energy, environmental and economic impacts of coal versus wood pellets for generating heat in China

Wang, C. *et al. Energy*, 2017, 120, 374–384.

This study investigated whether wood pellets were more sustainable than coal for heating buildings in China by presenting a 'fuel-to-heat' energy, environmental and economic comparison for both energy sources. Pellet and coal heating systems were modelled using a process-based life cycle inventory modelling approach, and the energy consumption and air pollutant emissions were calculated in gigajoules (GJ). Wood pellets were also analysed for their costs and market competitiveness against coal and other fossil fuel heating alternatives. The results showed that the energy saving potential from using pellets instead of coal was 1382 MJ for every 1-GJ of heat generated. Greenhouse gas emissions from pellets were 11.76 kg CO_2-eq GJ^{-1} heat, which were approximately 94% less than emissions from coal heating systems. Also, the wood pellet systems reduced SO_2, NO_x and PM emissions by 86%, 56% and 33%. However, the cost of pellets is significantly higher than the cost for coal, and is the primary impediment for the transition from coal to pellets in China. In addition, multiple consumers of wood residue, unstable heat values of pellet, limited supplies, and the lack of product and heating equipment standards also render the transition from coal to pellets impractical.

18/00590 Effect of pretreatment on microalgae pyrolysis: kinetics, biocrude yield and quality, and life cycle assessment

Wang, X. *et al. Energy Conversion and Management*, 2017, 132, 161–171.

Effects of three different cell pre-treatment methods on microalgae *Isochrysis* sp. pyrolysis kinetics, biocrude yields and quality, energy conversion efficiency and life cycle assessment (LCA) were investigated. From derived thermogrametry (DTG) curves, the decomposition reaction was apparently enhanced for acid pre-treatment sample at 200 °C. The activation energy of pre-treated microalgae pyrolysis was lower than that without pre-treatment. The biocrude yields for raw microalgae were higher than pre-treated samples at 450–475 °C and lower at 400–425 °C. Carbon distributions of biocrude from microalgae pyrolysis with ultrasonication and microwave pre-treatment were similar and mainly in C6-10, C16, C18 and C20, while carbon distribution of biocrude from acid pre-treatment mainly located in C7, C16, C18 and C20. Acid heating pre-treatment improved fuel quality including N compounds reduction and increase of esters and ethers content, which was likely due to esterification reaction between carbohydrate derivative and lipid at acid conditions. From the point of energy conversion efficiency, pre-treatment decreased the energy ratio and energy efficiency and increased the energy consumption/output ratio *ECR* (except *ECR* of acid heating pre-treatment) during microalgae pyrolysis process. Based on the LCA, pre-treatment increased the greenhouse gas emissions in the production process of alternative biofuels. Co-use of pre-treatment process during biofuel production and valuable chemicals extraction can be further researched to enhance energy efficiency and cost-efficiency for microalgae.

18/00591 Life cycle assessment of a mallee eucalypt jet fuel

Crossin, E. *Biomass and Bioenergy*, 2017, 96, 162–171.

This study uses life cycle assessment to quantify and compare the greenhouse gas emissions and fossil fuel depletion impacts of a theoretical mallee jet fuel value chain, operating in the Great Southern region of Western Australia, with those of fossil-based jet fuel. Relative to fossil-based jet fuel, the mallee jet fuel was found to reduce greenhouse gas emissions by 40% and result in a net fossil fuel depletion benefit. Further greenhouse gas reductions could be achieved by optimizing the supply chain through measures such as capturing methane emissions for hydrogen production and utilizing co-produced biodiesel. The magnitudes of the environmental benefits are sensitive to a number of methodology assumptions, including the approach to potential food displacement and co-production.

18/00592 Life cycle assessment of a medium commercial scale biogas plant and nutritional assessment of effluent slurry

Yasar, A. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 364–371.

This study addresses the life cycle assessment (LCA) of a novel design multi-digester anaerobic bioenergy plant. Notably the impacts regarding bioenergy generation and utilization of bioenergy and digestate are reviewed with reference to three different feed stocks used and experimented in this typical plant i.e. slurries of; 100% cow-dung, 75% cow-dung + 25% potato-pulp and 100% potato-pulp respectively. The results depicted that concentrations of nitrogen, phosphorus and potassium (NPK) and heavy metals (Cu, Ni, Mn and Fe) were highest in feedstock comprising 75% cow-dung + 25% potato-pulp. The comparative LCA of said feedstocks was further deliberated in three representative environmental impact categories, i.e. climate change potential (CO_2 equivalent), fresh-water eutrophication potential (Phosphorous equivalent) and acidification potential (SO_2 equivalent). The results revealed that feedstock comprising 100% cow-dung had highest savings in-terms of climate change, i.e. 70 kg, lowest acidification potential, i.e. 5 kg and considerably more fresh-water eutrophication potential, i.e. 0.022 kg. The second best proven feedstock was 100% potato-pulp having potentials regarding climate change, acidification and fresh-water eutrophication as: 70.5, 6.5 and 0.021 kg respectively. Whereas the feedstock comprising 75% cow-dung + 25% potato-pulp had the highest comparative life cycle impacts, i.e. 200, 6.9 and 0.034 kg against climate change, acidification and fresh-water eutrophication categories.

18/00593 Life cycle assessment of buildings and city quarters comparing demolition and reconstruction with refurbishment

Weiler, V. *et al. Energy and Buildings*, 2017, 134, 319–328.

In the building sector, the energy and the greenhouse gases embodied in the building materials are becoming increasingly important. Combined with the operational primary energy demand and the end-of-life, the whole life cycle of buildings can be assessed. In this paper, a comprehensive method for calculating the life cycle of individual buildings is presented. First, their material composition has been determined and generic values for the embodied energy, embodied greenhouse gases, energy needed and greenhouse gases emitted during disposal of the different building materials have been calculated. Subsequently these values have been integrated into an urban energy simulation software to simulate energy and emission values for buildings. A given building geometry with four different building standards was considered. The results can help to decide between building refurbishment or demolition and new construction. For example it could be shown that the share of the life cycle stage production compared to the total value rises with a better building insulation standard, as the share of the use stage decreases. The highest building refurbishment standard resulted in the best life cycle performance when compared with less ambitious refurbishment or construction of a new building of today's standards.

18/00594 Life cycle energy efficiency in building structures: a review of current developments and future outlooks based on BIM capabilities

Eleftheriadis, S. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 811–825.

The continuous developments of building information modelling (BIM) in architecture, engineering and construction (AEC) industry supported by the advancements in material resourcing and construction processes could offer engineers the essential decision-making procedures to leverage the raising demands for sustainable structural designs. This article brings together the theory of life cycle assessment (LCA) and the capabilities of BIM to survey the current developments in the energy efficiency of structural systems. In addition, the article explores the engineering dimensions of common decision-making procedures within BIM systems including optimization methods, buildability and safety constraints and code compliance limitations. The research presents critical expositions in both engineering and sustainable energy domains. The article then argues that future innovations in the sustainable decision-making of buildings' structures would require BIM-integrated workflows in order to facilitate the conflicting nature of both energy efficient and engineering performance indexes. Finally, the study puts forward a series of research guidelines for a consolidated decision paradigm that utilizes the capabilities of BIM within the engineering and sustainable energy domains in a synergistic manner.

18/00595 Streamlined life cycle analysis for assessing energy and exergy performance as well as impact on the climate for landfill gas utilization technologies
Friesenhan, C. *et al. Applied Energy*, 2017, 185, 805–813.
Three landfill gas (LFG) valorization technologies were compared using energy and exergy efficiency and a streamlined life-cycle assessment (LCA) method. The technologies were (i) steam reforming and hydrogen utilization in an *in situ* cogeneration fuel cell (SR-IS-FCC), (ii) biogas utilization in an *in situ* gas engine cogeneration plant (IS-GEC) and (iii) amine scrubbing and biomethane utilization in an *ex situ* gas engine cogeneration plant (AS-ES-GEC). The SR-IS-FCC alternative recorded the highest exergy efficiency and savings in cumulative energy demand (CED), and the lowest global warming potential (GWP) when all the heat is utilized *in situ*; otherwise, the highest exergy efficiency and the lowest GWP and CED were associated with the AS-ES-GEC alternative. The results indicate that AS-ES-GEC is the preferential choice when heat cannot be utilized *in situ*. Otherwise, SR-IS-FCC records the best values for the three criteria, and the AS-ES-GEC technology is the least interesting alternative.

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Supplies, policy, economics, forecasts

18/00596 A dynamic programming approach for modeling low-carbon fuel technology adoption considering learning-by-doing effect
Chen, Y. *et al. Applied Energy*, 2017, 185, 825–835.
Promoting the adoption of low-carbon technologies in the transportation fuel portfolio is an effective strategy to mitigate greenhouse gas emissions from the transportation sector worldwide. However, as one of the most promising low-carbon fuels, cellulosic biofuel has not fully entered commercial production. Governments could provide guidance in developing cellulosic biofuel technologies, but no systematic approach has been proposed yet. The authors establish a dynamic programming framework for investigating time-dependent and adaptive decision-making processes to develop advanced fuel technologies. The learning-by-doing effect inherited in the technology development process is included in the framework. The proposed framework is applied in a case study to explore the most economical pathway for California to develop a solid cellulosic biofuel industry under its Low Carbon Fuel Standard. The results show that cellulosic biofuel technology is playing a critical role in guaranteeing California's 10% greenhouse gas emission reduction by 2020. Three to 4 billion gallons of cumulative production are needed to ensure that cellulosic biofuel is cost-competitive with petroleum-based fuels or conventional biofuels. Zero emission vehicle promoting policies will discourage the development of cellulosic biofuel. The proposed framework, with small adjustments, can also be applied to study new technology development in other energy sectors.

18/00597 A hybrid BAG-SA optimal approach to estimate energy demand of China
Wu, Q. and Peng, C. *Energy*, 2017, 120, 985–995.
To improve projection efficiency of future energy demand, this paper proposes a hybrid optimization method, which is bat algorithm, Gaussian perturbations and simulated annealing energy demand estimation (BAG-SA EDE) model. The proposed BAG-SA algorithm not only inherits the simplicity and efficiency of the standard BA with a capability of searching for global optimality, but also enhances local search ability and speeds up the global convergence rate. The causality of energy demand and the selected factors is further investigated via the Stationarity, Cointegration and Granger causality tests. Then, BAG-SA algorithm is employed to optimize the coefficients of multiple linear and quadratic equations of energy demand estimation models. Results indicate that the proposed algorithm has higher precision and reliability than other single optimization methods, such as genetic algorithm, particle swarm optimization or bat algorithm, and the quadratic form of BAG-SA EDE model has better fitting ability compared with the multiple linear form of the model. Therefore, the quadratic form of the model is applied to estimate energy demand of China from 2016 to 2030 in dissimilar scenarios. The forecasting findings show that energy demand in 2030 will be 4.6, 6.1 and 7.9 billion tce in three scenarios.

18/00598 A review and assessment of energy policy in the Middle East and North Africa region
Griffiths, S. *Energy Policy*, 2017, 102, 249–269.
The energy landscape of the Middle East and North Africa (MENA) region has undergone a significant transformation in recent years as a result of intersecting technological, economic and political trends, both regional and international. The evolving dynamics of international energy markets, increased diversification of energy sources, global concerns for climate change, and regional conflict are among the leading factors impacting the evolution of MENA energy policy. This paper provides an assessment and outlook for energy policy in the MENA region within the context of the myriad factors impacting policy design and implementation. A review and analysis of the social, political and economic factors that are impacting regional energy policy is provided and followed by analysis of regional energy policy with consideration of hydrocarbon exploration and production, regional energy trade, demand management and clean energy production. The findings show that the MENA region is in the midst of an energy transition that has uncertain outcomes but will undoubtedly have long lasting impacts on the global energy system.

18/00599 A review of the bandwidth and environmental discourses of future energy scenarios: shades of green and gray
Laugs, G. A. H. and Moll, H. C. *Renewable and Sustainable Energy Reviews*, 2017, 67, 520–530.
Energy scenarios are often used to investigate various possible energy futures and reduce the uncertainty that surrounds energy transition. However, scenario construction lacks consistent and adequate methodological standards, resulting in limited insight into the actual bandwidth covered by current energy scenarios and whether various perspectives on future energy development pathways are all adequately represented. This research deployed a non-mathematical clustering approach to identify general trends in future energy scenarios and assess the role of Cornucopian and Malthusian oriented world views therein. It was found that the futures communicated in quantified future energy scenarios overlap to a large extent and represent only a narrow bandwidth of moderate world views. It is argued that the underrepresentation of extreme representations of world views and environmental discourses in energy scenarios skews the overall outlook on possible energy futures. This implies that scenario-informed policy design and decision-making risks bias towards the status-quo.

18/00600 An estimation of the effect of carbon pricing for CO_2 mitigation in China's cement industry
Liu, X. *et al. Applied Energy*, 2017, 185, 671–686.
This study estimates the effect of carbon pricing for CO_2 mitigation in China's cement industry. The statistics and prediction show that cement production initially experienced accelerated growth and is now expected to plateau out over the next few years. The energy saving and carbon mitigation technologies considered in this estimation are at different adoption stages. Full technology diffusion is expected within 10–20 years, and the remaining technology mitigation potential stands at about 8.8% by 2025 and 10.2% by 2030. Nevertheless, attaching a price to carbon would have a limited effect. Reductions of 9.9 and 12.9 Mt-CO_2 might have been realized in 2015 under respective prices of 60 and 100 Yuan/t-CO_2, compared to a non-pricing scenario. The reduction attributed to carbon pricing would be around 4.9 Mt-CO_2 in 2020 at both price levels, and around 70% of the mitigation may be at a marginal cost of 50 Yuan/t-CO_2 by 2020. The marginal cost for nearly 90% of the policy mitigation would be below 100 Yuan/t-CO_2 by 2030. This paper confirms the effectiveness of a command-and-control approach so far for energy saving in China's cement industry and advises early introduction of a carbon pricing regime with consideration of policy interactions.

18/00601 An expert knowledge based decommissioning alternative selection system for fixed oil and gas assets in the South China Sea
Na, K. L. *et al. Ocean Engineering*, 2017, 130, 645–658.
The decommissioning process is constantly challenged with indeterminate risks associated with deteriorated structures and the practice of late-life decommissioning planning. The issue is further complicated by the absence of a fit-for-purpose decision framework. This work develops a knowledge based advisory expert system to address the late-life structural ambiguity of fixed jacket platforms in the selection of a best practicable decommissioning method. A review on the decommissioning industry and its growing need for data-driven management are presented. Analytic hierarchy process is utilized to solve the multi-criteria decision making problem of choosing the best practicable decommissioning alternative. The effects and ranking of identified key structural-operation factors on the decommissioning planning process are numerically computed and discussed. The key system variables are developed with reference to established Asset Integrity Management Systems. Subject matter expert surveys are

conducted on leading decommissioning and structural integrity experts in the region which are reflected in the decision matrices. A mathematical standardization technique is employed to remove inconsistencies in the intermediate decision vectors. The model is benchmarked against an actual decommissioning project in Malaysian waters which was based on conventional practices. A comprehensive framework is proposed to establish a practical working philosophy for the developed algorithm.

18/00602 Analyzing sustainability in low-income housing projects using system dynamics

Marzouk, M. and Azab, S. *Energy and Buildings*, 2017, 134, 143–153.

Low-income housing (LIH) projects have a vital role in developing countries as they serve a large sector of society; hence, they are considered one of the most important projects funded by governments. The total life-cycle cost (LCC) of these projects is incurred during the use phase, making these projects lose its economic aspect of sustainability. Therefore, it is important to decrease the costs of such projects during their life cycle, taking into consideration the available resources. This paper focuses on two aspects of the sustainability of building through its life cycle; environmental and economic. For this purpose, the methodology considers reasonable costs that fit LIH projects using environmentally friendly materials. The methodology is based on assessing the LCC of LIH projects, taking into consideration initial cost and operation costs. The paper focuses on green-building materials with minimal cost, corresponding to the maximum number of points awarded under the leadership in energy and environmental design (LEED) rating system. This methodology is developed through the formulation of the system dynamics (SD) model using a STELLA software package. The proposed model is capable of considering the dynamic nature and interactions among major variables affecting the assessment of economic and environmental performances of selected green materials. The proposed assessment methodology helps the decision makers in governmental housing authorities to modify the current management policies for improving the current situation of LIH. In addition, it aids government and/or contractors to minimize LCC while achieving maximum LEED material credit points for LIH projects. A detailed case study in Egypt is presented to clarify the practical features of the proposed model.

18/00603 Energy consumption, inter-fuel substitution and economic growth in Nigeria

Lin, B. and Atsagli, P. *Energy*, 2017, 120, 675–685.

Nigeria's energy mix has been dominated by petroleum with a year on year increase due to huge petroleum subsidy by the government. This study adopts the translog production function to investigate the potential for inter-factor and inter-fuel substitution between capital, labour, petroleum and electricity. Ridge regression has been adopted to estimate the model's parameters due to evidence of multicollinearity in the data. The results show that all input pairs are substitutes; and as such, adopting competitive pricing policies and removal of petroleum subsidies and price ceilings would redirect industries towards an increased use of electricity and increase capital and labor intensiveness. In addition, the study shows that a 5% and 10% increase of investment in petroleum reduction technologies for the period 2010, 2011 and 2012 would reduce CO_2 emissions by 1.13518, 1.8554, 1.2722 and 2.27119, 2.37109, 2.49444 million metric tons, respectively. Furthermore, the study points to evidence for convergence in relative technical progress among the various input pairs with electricity registering the fastest rate. These imply that petroleum would gradually lose its dominance in Nigerian energy mix.

18/00604 Energy price, regulatory price distortion and economic growth: a case study of China

Shi, X. and Sun, S. *Energy Economics*, 2017, 63, 261–271.

Energy prices are often distorted by government control, which is justified on the grounds that such control will help mitigate the negative impact of price volatility from oil imports, and thus positively affect the domestic economy. This paper shows, in a two-sector growth model, that regulatory price distortion can negatively affect the economy. Based on the model, the authors then empirically estimate the impact of the price distortion on output growth in China, using monthly, time series data from 2005M1 to 2012M12. In contrast to the usual argument for regulatory control to mitigate price volatility, it was found that regulatory price distortion negatively affects output growth in China during both the short and long term, because it is robust to different measures of output and price distortion. Hence, the argument that using price regulation to protect economic growth is undermined, and subsequently, this study lends its support to energy price deregulation. A market oriented energy price regime may improve the resilience of the domestic economy to global oil price shocks.

18/00605 European smart grid prospects, policies, and challenges

IqtiyaniIlham, N. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 776–790.

A smart grid (SG) is developed to overcome grid congestion and to meet the demand for and sustain the supply of electricity. The European SG is supported by European Union (EU) policies and the joint EU Energy and Climate Package. This study reviews the prospects, progress, policies, and challenges faced by EU countries, electricity networks, and their relevant stakeholders. European SG prospects were initiated through the EU's Strategic Energy Technologies plan and continue with the strategic research agenda that has been road-mapped for 2007–2035. The EU, with its directorates-general, agencies, and commissions, has established directives and policies to promote SG among member states. The factors that stimulate the innovation and implementation of SG require the need to generate electricity optimally (i.e. low greenhouse gas emission and renewable or sustainable source) and to secure its supply while ensuring reliability and quality. Despite the challenges, the European SG continues to develop and progress, fulfilling renewable energy targets and customer satisfaction and addressing environmental concerns.

18/00606 Evidence of direct and indirect rebound effect in households in EU-27 countries

Freire-González, J. *Energy Policy*, 2017, 102, 270–276.

This research estimates the direct and indirect rebound effect of energy efficiency in households for the EU-27 countries (the first 27 member states of the EU). A hybrid methodology that combines econometric estimates, environmental extended input-output analysis and re-spending models has been developed. Although most of the economies present values below 100%, there are seven countries situated above this critical threshold. By weighting individual estimates by GDP, an average value for the overall EU-27 economy has been found between 73.62% and 81.16%. These results suggest that the energy policy at the European level should be rethought if efficiency measures pursue reducing energy consumption and tackling climate change.

18/00607 Financial stability, energy consumption and environmental quality: evidence from South Asian economies

Nasreen, S. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 1105–1122.

A few studies are found on the relationship between financial instability, energy consumption and environmental quality in energy economics literature. The current study is an endeavour to fill this gap by investigating the relationship between financial stability, economic growth, energy consumption and carbon dioxide (CO_2) emissions in South Asian countries over the period 1980–2012 using a multivariate framework. Bounds test for cointegration and Granger causality approach are employed for the empirical analysis. Estimated results suggest that all variables are non-stationary and cointegrated. The results show that financial stability improves environmental quality; while the increase in economic growth, energy consumption and population density are detrimental for environment quality in the long-run. The results also support the environmental Kuznets curve (EKC) hypothesis which assumes an inverted U-shaped path between income and environmental quality. Moreover, the study found the evidence of unidirectional causality running from financial stability to CO_2 emissions in two countries, i.e. Pakistan and Sri Lanka. The findings of this study open up new insight for policy makers to design a comprehensive financial, economic and energy supply policies to minimize the detrimental impact of environmental pollution.

18/00608 Hazard tolerance of spatially distributed complex networks

Dunn, S. and Wilkinson, S. *Reliability Engineering & System Safety*, 2017, 157, 1–12.

This paper presents a new methodology for quantifying the reliability of complex systems, using techniques from network graph theory. In recent years, network theory has been applied to many areas of research and has allowed us to gain insight into the behaviour of real systems that would otherwise be difficult or impossible to analyse, for example increasingly complex infrastructure systems. Although this work has made great advances in understanding complex systems, the vast majority of these studies only consider a systems topological reliability and largely ignore their spatial component. It has been shown that the omission of this spatial component can have potentially devastating consequences. In this paper, the authors propose a number of algorithms for generating a range of synthetic spatial networks with different topological and spatial characteristics and identify real-world networks that share the same characteristics. They assess the influence of nodal location and the spatial distribution of highly connected nodes on hazard tolerance by comparing the generic networks to benchmark networks. The relevance of these findings are discussed for real world

networks and it is shown that the combination of topological and spatial configurations renders many real world networks vulnerable to certain spatial hazards.

18/00609 How do policies for efficient energy use in the household sector induce energy-efficiency innovation? An evaluation of European countries

Girod, B. *et al. Energy Policy*, 2017, 103, 223–237.

Research on innovation induced by climate-mitigation policy has been focused predominantly on the supply side of the energy system. Despite considerable climate-mitigation potential on the demand side, less attention is given to the innovation effect of policies addressing the household sector. Based on a comprehensive data set, including 550 policy measures over 30 years (1980–2009) and covering 21 European countries,the authors found – based on econometric estimations – that policies targeting efficient energy use in the household sector significantly increase the number of patented energy-efficiency inventions. A comparison of the different policy types reveals a particularly strong influence from financial subsidies and energy labels. The results indicate that policies supporting early market adoption of energy-efficient technologies are effective in fostering innovation.

18/00610 How to enhance the future use of energy policy simulation models through ex post validation

Qudrat-Ullah, H. *Energy*, 2017, 120, 58–66.

Although simulation and modelling in general and system dynamics models in particular has long served the energy policy domain, *ex post* validation of these energy policy models is rarely addressed. In fact, *ex post* validation is a valuable area of research because it offers modellers a chance to enhance the future use of their simulation models by validating them against the field data. This paper contributes by presenting (i) a system dynamics simulation model, which was developed and used to do a three-dimensional, socio-economic and environmental long-term assessment of Pakistan's energy policy in 1999, (ii) a systematic analysis of the 15-year-old predictive scenarios produced by a system dynamics simulation model through *ex post* validation. How did the model predictions compare with the actual data? The authors report that the ongoing crisis of the electricity sector of Pakistan is unfolding, as the model-based scenarios had projected.

18/00611 Impact of political and economic barriers for concentrating solar power in Sub-Saharan Africa

Labordena, M. *et al. Energy Policy*, 2017, 102, 52–72.

Sub-Saharan Africa (SSA) needs additional affordable and reliable electricity to fuel its social and economic development. Ideally, all of this new supply is carbon-neutral. The potentials for renewables in SSA suffice for any conceivable demand, but the wind power and photovoltaic resources are intermittent and difficult to integrate in the weak electricity grids. Here, the authors investigate the potential for supplying SSA demand centres with dispatchable electricity from concentrating solar power (CSP) stations equipped with thermal storage. They show that, given anticipated cost reductions from technological improvements, power from CSP could be competitive with coal power in Southern Africa by 2025; but in most SSA countries, power from CSP may not be competitive. The authors also show that variations in risk across countries influences the cost of power from CSP more than variations in solar resources. If policies to de-risk CSP investment to financing cost levels found in industrialized countries were successfully implemented, power from CSP could become cheaper than coal power by 2025 in all SSA countries. Policies to increase institutional capacity and cooperation among SSA countries could reduce costs further. With dedicated policy measures, therefore, CSP could become an economically attractive electricity option for all SSA countries.

18/00612 Integrating water and energy models for policy driven applications. A review of contemporary work and recommendations for future developments

Khan, Z. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 1123–1138.

Availability of and access to water and energy are key ingredients for economic and social development. Unfortunately, more than a billion people still lack access to both safe freshwater and basic energy services. Future predictions show that the situation may become worse with about a 40% increase in energy demand and 30% increase in water demand by 2040. In addition, water and energy are highly interdependent, with water needed in all phases of the energy lifecycle and energy needed in all phases of the water lifecycle. While recent years have seen an increasing number of studies on the water-energy nexus, the research is focused on scattered individual areas of the nexus, each important in their own right. However, there is now a need to synthesize these efforts and identify the most important elements needed for a holistic water-energy nexus methodology. This paper focuses on the benefits to be gained from and the drawbacks of ignoring various water-energy interlinks for policy makers and planners in their goals to meet long term resource security. Several possible combinations of socio-economic and climate change scenarios make these goals even more challenging. The lessons learnt from reviewing different integration methodologies and studies are compiled into a list of key recommendations. It is found that current integration efforts are often biased towards the energy sector and its water requirements. There is still a need for better representations of the water infrastructure and corresponding linkages with the energy sector. There is also a need to harmonize the energy and water systems from both a technical and policy perspective. This calls for compatible disaggregation of spatial and temporal elements in both systems as well as designing model outputs to allow evaluation of the synergies and trade-offs of multi-scale, cross-sector policies.

18/00613 Interpreting Turkish industry's perception on energy security: a national survey

Biresselioglu, M. E. *et al. Renewable and Sustainable Energy Reviews*, 2017, 67, 1208–1224.

Along with the changing concerns over energy security in the last decades, it is important to investigate the perception of different segments of society in order to understand how they view the challenges and opportunities in contemporary energy issues. Being one of the most dynamic energy economies globally, Turkey is continuously increasing both its electricity generation and consumption. Since the industrial sector accounts for higher ratios in this growth, this article explores the perception and awareness within Turkish industrial companies related to energy security, Turkish energy policy, and compatibility of corporate strategy with governmental energy and industrial policies. The study is based on the exploration of nine suppositions relating to the following issues: importance of energy costs in supply chain management, energy efficiency priority, effectiveness of legal infrastructure for energy efficiency, import dependency awareness, renewable energy awareness, the compatibility of energy strategy, climate change awareness, the level of Kyoto Protocol awareness, and compatibility between firm-specific targets and strategy papers. The study tests these suppositions with a survey based on the existing academic literature and three strategy documents related to industrial and energy policies, namely papers on Energy Efficiency Strategy, Turkish Industrial Strategy, and Electricity Energy Market and Security of Supply Strategy. These papers provide the research background and give insight for each of the suppositions. A survey was distributed to the top 500 Turkish industrial companies listed in ISO500. The results show that six suppositions are supported, one is unsupported, and two is neither supported nor unsupported.

18/00614 Is information assimilated at announcements in the European carbon market?

Chen, J. *et al. Energy Economics*, 2017, 63, 234–247.

This study examines the high frequency new information impact on prices, volatility, trading volume and illiquidity at scheduled macroeconomic and verified emissions announcements for the European carbon futures market. Verified emissions, US non-farm payroll and German new factory order macroeconomic announcements impact carbon prices swiftly, within 5 min. The authors show that a one standard deviation surprise increase in verified emission announcements is associated with an approximate ten percentage point (9.96%) increase in carbon futures returns. A wait-and-see stylized trading behaviour is evident at announcements in volatility and trading volumes. Market illiquidity increases at announcements in relation to US non-farm payroll, albeit there is no evidence of an increase in illiquidity prior to announcements. The development of new information impact, over time, occurs mainly in the at-announcement 5-minute time interval.

18/00615 Marine spatial planning as a tool for regional ocean governance?: an analysis of the New England ocean planning network

Smythe, T. C. *Ocean & Coastal Management*, 2017, 135, 11–24.

Marine spatial planning (MSP) requires extensive integration and collaboration between and among government agencies and non-governmental individuals and organizations. Such collaboration has also been identified as critical to the broader goal of achieving regional ocean governance. Social network analysis (SNA) is a suite of methods for systematically analysing relations between individuals and organizations and provides insight into the extent and nature of collaboration and into governance networks more broadly. A SNA was conducted of the governance network shaping a regional MSP initiative in the New England region of the USA from 2012 to 2014, focusing in particular on a subset of key collaborators comprising the core of this network. The SNA was designed to investigate whether this network demonstrates the level of inter-organizational collaboration and integration that MSP scholars assert is needed to meaningfully improve regional ocean governance. Results suggest that the broader New England regional ocean planning network is large, decentralized, and of low density, thus well-suited to solving complex boundary-spanning

problems like the management of ocean space. The core collaboration network is similarly diverse; well-connected and influential members of the core collaboration network include representatives of intergovernmental regional ocean partnerships, state government affiliates, and, to a lesser extent, federal government affiliates. Influential members also include key representatives of non-governmental organizations and universities. Conversely, local government affiliates are absent from the network, and ocean users and industry representatives are also absent from the core collaboration network but are included in the broader network and involved in the MSP process through targeted outreach efforts. These results indicate that both horizontal and vertical collaboration are being facilitated through the core collaboration network, though collaboration could be improved through greater participation by local government, users, and industry. This study illustrates how MSP, applied regionally, may help facilitate collaboration, thereby helping to advance a regional ocean governance approach, but that further research is needed to compare this case to others and to observe how this network sustains over time.

18/00616 Multi-criteria ranking of energy generation scenarios with Monte Carlo simulation

Baležentis, T. and Streimikiene, D. *Applied Energy*, 2017, 185, 862–871.
Integrated assessment models (IAMs) are omnipresent in energy policy analysis. Even though IAMs can successfully handle uncertainty pertinent to energy planning problems, they render multiple variables as outputs of the modelling. Therefore, policy makers are faced with multiple energy development scenarios and goals. Specifically, technical, environmental, and economic aspects are represented by multiple criteria, which, in turn, are related to conflicting objectives. Preferences of decision makers need to be taken into account in order to facilitate effective energy planning. Multi-criteria decision making (MCDM) tools are relevant in aggregating diverse information and thus comparing alternative energy planning options. The paper aims at ranking European Union (EU) energy development scenarios based on several IAMs with respect to multiple criteria. By doing so, the authors account for uncertainty surrounding policy priorities outside the IAM. In order to follow a sustainable approach, the ranking of policy options is based on EU energy policy priorities: energy efficiency improvements, increased use of renewables, reduction in and low mitigations costs of GHG emission. The ranking of scenarios is based on the estimates rendered by the two advanced IAMs relying on different approaches, namely TIAM and WITCH. The data are fed into the three MCDM techniques: the method of weighted aggregated sum/product assessment (WASPAS), the additive ratio assessment (ARAS) method, and technique for order preference by similarity to ideal solution (TOPSIS). As MCDM techniques allow assigning different importance to objectives, a sensitivity analysis is carried out to check the impact of perturbations in weights upon the final ranking. The rankings provided for the scenarios by different MCDM techniques diverge, first of all, due to the underlying assumptions of IAMs. Results of the analysis provide valuable insights in integrated application of both IAMs and MCDM models for developing energy policy scenarios and decision making in energy sector.

18/00617 Policy design for controlling set-point temperature of ACs in shared spaces of buildings

Tushar, W. *et al. Energy and Buildings*, 2017, 134, 105–114.
Air conditioning (AC) systems are responsible for the major percentage of energy consumption in buildings. Shared spaces constitute considerable office space area, in which most office employees perform their meetings and daily tasks, and therefore the ACs in these areas have significant impact on the energy usage of the entire office building. The cost of this energy consumption, however, is not paid by the shared space users, and the AC's temperature set-point is not determined based on the users' preferences. This latter factor is compounded by the fact that different people may have different choices of temperature set-points and sensitivities to change of temperature. Therefore, it is a challenging task to design an office policy to decide on a particular set-point based on such a diverse preference set. As a consequence, users are not aware of the energy consumption in shared spaces, which may potentially increase the energy wastage and related cost of office buildings. In this context, this paper proposes an energy policy for an office-shared space by exploiting an established temperature control mechanism. In particular, the authors chose meeting rooms in an office building as the test case and designed a policy according to which each user of the room can give a preference on the temperature set-point and is 'paid' for feeling discomfort if the set-point is not fixed according to the given preference. On the other hand, users who enjoy the thermal comfort compensate the other users of the room. Thus, the policy enables the users to be cognizant and responsible for the 'payment' on the energy consumption of the office space they are sharing, and at the same time ensures that the users are satisfied either via thermal comfort or through incentives. The policy is also shown to be beneficial for building management. Through experiment based case studies, the effectiveness of the proposed policy is shown.

18/00618 Price and income elasticities of residential energy demand in Germany

Schulte, I. and Heindl, P. *Energy Policy*, 2017, 102, 512–528.
This study applies a quadratic expenditure system to estimate price and expenditure elasticities of residential energy demand (electricity and heating) in Germany. Using official expenditure data from 1993 to 2008, the authors estimate an expenditure elasticity for electricity of 0.3988 and of 0.4055 for space heating. The own price elasticity for electricity is −0.4310 and −0.5008 in the case of space heating. Disaggregation of households by expenditure and socio-economic composition reveals that the behavioural response to energy price changes is weaker (stronger) for low-income (top-income) households. There are considerable economies of scale in residential energy use but scale effects are not well approximated by the new OECD equivalence scale. Real increases in energy prices show a regressive pattern of incidence, implying that the welfare consequences of direct energy taxation are larger for low income households. The application of zero-elasticities in assessments of welfare consequences of energy taxation strongly underestimates potential welfare effects. The increase in inequality is 22% smaller when compared to the application of disaggregated price and income elasticities as estimated in this paper.

18/00619 Prospects for Chinese electric vehicle technologies in 2016–2020: ambition and rationality

Du, J. *et al. Energy*, 2017, 120, 584–596.
As the world's largest market for vehicles, China is facing challenges related to energy security and urban air pollution. The development of electric vehicles has been determined to be the national strategy for solving these problems. By the end of 2015, China had become the world's largest electric vehicles market, but its core technologies are still less competitive in the global marketplace. A scientific national strategy for 2016–2020 is expected to play a critical role in China becoming the global leader in the electric vehicle industry. The research process for this strategy includes a review of the technologies for electric vehicles, market analyses, benchmarking of the top levels in the field, and expert interviews. By these approaches, the strengths and weaknesses of China's electric vehicle technologies and industry are assessed. Competitive and feasible quantitative goals for key components and powertrains are proposed by this paper, and a core issue has been determined to be the need to improve the safety of high-energy density traction batteries. Improving the power density of electric control units is expected to the core for electric vehicles' electronics and control systems. Key problems for the fuel cell stacks used in cars and buses have been identified by this paper to be, respectively, power density and durability. Long-range plug-in hybrid electric powertrains are the optimal candidate for Chinese plug-in hybrid electric vehicles. Lightweight material, intelligent driving technologies and special electric chassis are set to be the focus for improving the energy efficiency of battery electric vehicles. Comprehensive safety and recyclable electric vehicle technologies are set to become key issues in the future, and the Chinese government should research and develop these in advance.

18/00620 Rationales for technology-specific RES support and their relevance for German policy

Gawel, E. *et al. Energy Policy*, 2017, 102, 16–26.
In order to achieve cost-effective electric power generated from renewable energy sources (RES-E) deployment it is often argued that technology-neutral support schemes for renewables are indispensable. Against this background, RES-E support policies making widely use of technology differentiation in remuneration settings, e.g. across the EU, are frequently criticized from a theoretical point of view. However, this paper provides a systematic critique of the technology neutrality concept as a foundation for designing policy support schemes in the RES-E technology field. Specifically, the main objective of the paper is to scrutinize the arguments for technology-neutrality, and discuss three conceptual arguments for why technology-specific support schemes could in fact help minimize the societal costs of reaching future RES-E targets. This paper also briefly addresses different political economy concerns, which could constrain the choice of cost-effective policy support schemes, and that have to be taken into account for economic policy advice. For an empirical illustration of the key arguments, the authors refer to the case of German RES-E policy-making. The central conclusion from this paper is that technology-specific RES-E support schemes may generate significant economic benefits, particularly if technology markets work imperfectly and in second-best policy settings with additional non-internalized market failures.

18/00621 The effect of learning on climate policy under fat-tailed risk

Hwang, I. C. *et al. Resource and Energy Economics*, 2017, 48, 1–18.

This paper investigates the effect of learning on climate policy under fat-tailed risk about climate change. An endogenous learning model with fat-tailed uncertainty about the equilibrium climate sensitivity was constructed. It was found that a decision maker with a possibility of learning lowers efforts to reduce carbon emissions relative to the no-learning case. The larger the tail effect, the larger the counteracting learning effect because learning reduces the marginal benefit of emissions control compared to the case where there is no learning. The optimal decisions (summarized by the carbon tax level) in the learning case are less sensitive to the true value of the uncertain variable than the decisions in the uncertainty case. Learning lets uncertainty converge to the true value of the state in the sense that the variance approaches zero as information accumulates.

18/00622 Vessels fuel consumption forecast and trim optimisation: a data analytics perspective

Coraddu, A. *et al. Ocean Engineering*, 2017, 130, 351–370.

In this paper, the authors investigate the problems of predicting the fuel consumption and of providing the best value for the trim of a vessel in real operations based on data measured by the on-board automation systems. Three different approaches for the prediction of the fuel consumption are compared: white, black and gray box models. White box models (WBM) are based on the knowledge of the physical underlying processes. Black box models (BBMs) build on statistical inference procedures based on the historical data collection. Finally, the authors propose two different gray box models (GBM) which are able to exploit both mechanistic knowledge of the underlying physical principles and available measurements. Based on these predictive models of the fuel consumption a new strategy for the optimization of the trim of a vessel is proposed. Results on real world operational data show that the BBM is able to remarkably improve a state-of-the-art WBM, while the GBM is able to encapsulate the *a priori* knowledge of the WBM into the BBM so to achieve the same performance of the latter but requiring less historical data. Moreover, results show that the GBM can be used as an effective tool for optimizing the trim of a vessel in real operational conditions.

18/00623 What policy adjustments in the EU ETS truly affected the carbon prices?

Fan, Y. *et al. Energy Policy*, 2017, 103, 145–164.

Carbon market becomes increasingly popular as a cost-effective instrument to mitigate CO_2 emissions. However, its construction is a learning-by-doing process, and needs consistent regulatory updates in order to deliver optimal effects. This paper uses the event study method to assess the impacts of different policy adjustments on the EU Allowance (EUA) returns in the EU emissions trading scheme (EU ETS) since 2005. Comparing to existing studies that focus on the impact of a single policy, this paper provides a complementary reference on if and to what extent policy adjustments can impact the carbon prices by classifying all regulatory update events into six categories. Its key findings are as follows. First, aggregate impacts of total 50 events studied are low while impacts of events having underlying negative impacts are higher than those having underlying positive impacts. Second, 24 events have significant impacts on EUA returns and are coherent to their theoretical impacts (except one event). Third, events having negligible impact on EUA returns are those that are announced not for the first time or those having no impact on CO_2 quotas supply and demand. Finally, there are different impact patterns: some events have different impacts on short-end and long-end carbon prices.

Energy conservation

18/00624 A new retrofit approach to the absorption-stabilization process for improving energy efficiency in refineries

Liu, X. G. *et al. Energy*, 2017, 118, 1131–1145.

In a refining complex, an absorption-stabilization process used in the production of end-use petro-products (i.e. stable gasoline and liquefied petroleum gas) is energy-intensive and costly. A new absorption-stabilization process with a two-stage condensation section is introduced in this work to further improve energy-use performance. In the new process, a condenser, a condensed oil tank, and a side-reboiler are integrated into the original process and then a heat integration scheme is performed. Compared with the existing process, the proposed process can reduce the cold utility and hot utility by 17.98% and 25.65%, respectively, as well as decrease the total annual operating costs of the heat exchanger network by 17.48%. Additionally, the process retrofit reduces the annual operating costs of cooling water and steam by about $346,617 at the expense of capital costs around $487,006, and the corresponding payback period is approximately 17 months.

18/00625 A novel method for optimal fuel consumption estimation and planning for transportation systems

Wörz, S. and Bernhardt, H. *Energy*, 2017, 120, 565–572.

With increasing public concern about the environment, liveability and sustainability have become important issues in minimal fuel consumption estimation for transportation systems. Microscopic fuel planning and emission models use vehicle speed and acceleration as inputs and are suitable for predicting the amount of fuel at the link level. However, the lack of microscopic traffic data limits the application of these models. A method is provided for acquiring microscopic information from macroscopic traffic data. The main approach is to reconstruct the state and vehicle group trajectories with an Expectation Maximization algorithm with nice convergence properties and then to apply Dijkstra's algorithm in order to find a transport route with minimal fuel consumption. Validation of the method shows that the estimated fuel consumption reflects the real fuel amount and hence, the route with minimal fuel consumption determined by Dijkstra's algorithm is actually suitable for optimal transport planning.

18/00626 Analysis of energy saving performance for household refrigerator with thermal storage of condenser and evaporator

Cheng, W.-l. *et al. Energy Conversion and Management*, 2017, 132, 180–188.

The heat transfer performances of evaporators and condensers significantly affect the efficiency of household refrigerators. For enhancing heat transfer of the condensers and evaporators, a novel dual energy storage (DES) refrigerator with both heat storage condenser (HSC) and cold storage evaporator (CSE) is proposed. The performance comparison of three kinds of energy storage refrigerators: HSC refrigerator, CSE refrigerator and DES refrigerator is analysed by establishing dynamic simulation models. According to the simulation results, the DES refrigerator combines the advantage of HSC refrigerator and CSE refrigerator, it has more balanced operational cycle and higher evaporation pressure and temperature. The DES refrigerator shows a best energy saving performance among the three energy storage refrigerators with largest off-time to on-time ratio of 4.3 and the electrical consumption saving can reach 32%, which is greater than the sum (28%) of the other two kinds of energy storage refrigerators.

18/00627 Benefits and risks of smart home technologies

Wilson, C. *et al. Energy Policy*, 2017, 103, 72–83.

Smart homes are a priority area of strategic energy planning and national policy. The market adoption of smart home technologies (SHTs) relies on prospective users perceiving clear benefits with acceptable levels of risk. This paper characterises the perceived benefits and risks of SHTs from multiple perspectives. A representative national survey of UK homeowners ($n = 1025$) finds prospective users have positive perceptions of the multiple functionality of SHTs including energy management. Ceding autonomy and independence in the home for increased technological control are the main perceived risks. An additional survey of actual SHT users ($n = 42$) participating in a smart home field trial identifies the key role of early adopters in lowering perceived SHT risks for the mass market. Content analysis of SHT marketing material ($n = 62$) finds the SHT industry are insufficiently emphasizing measures to build consumer confidence on data security and privacy. Policymakers can play an important role in mitigating perceived risks, and supporting the energy-management potential of a smart-home future. Policy measures to support SHT market development include design and operating standards, guidelines on data and privacy, quality control, and *in situ* research programmes. Policy experiences with domestic energy efficiency technologies and with national smart meter roll-outs offer useful precedents.

18/00628 Building scenarios for energy consumption of private households in Germany using a multi-level cross-impact balance approach

Vögele, S. *et al. Energy*, 2017, 120, 937–946.

A major goal concerning the energy transition in Germany is the reduction of energy usage. In Germany in 2011, private households consumed 2194 PJ and have been identified as a sector with high energy reduction potential. The energy demand of this sector is dependent on many linked quantitative and qualitative factors (e.g. number of persons and demographic structure, expenditures, cost of energy-saving measures, willingness to invest, and level of coordination in international climate policy). This study introduces a multilevel cross-impact approach which allows for the definition and quantification of data for scenario analysis while taking the interdependences between different factors on the global, national and sectoral levels into account. This approach makes it possible to overcome limitations that

conventional energy models are usually confronted with. By applying a trend analysis in combination with information on the interdependence of relevant factors on the global and national levels, consistent sectoral views of the private household's future are created.

18/00629 Cross-cultural assessment of the effectiveness of eco-feedback in building energy conservation

Ma, G. *et al. Energy and Buildings*, 2017, 134, 329–338.

To reduce energy consumption in buildings, researchers have in the recent decade explored the potential of changing occupants' energy consumption behaviours using eco-feedback technologies. Energy consumption behaviour is a type of consumer behaviour, which has been proven culture-specific in prior research. This paper aims to assess the impact of culture on the effectiveness of eco-feedback technologies in reshaping building occupants' energy consumption behaviours, and to examine the mechanism of such impact. A total of 39 students from 10 different countries who shared four university dormitories were recruited in an experiment. A web-based eco-feedback system was developed in this study, and implemented in these dormitories. The eco-feedback system was responsible for sending weekly email reminders to students participating in the study and, upon their login, providing them with their detailed energy consumption data as well as those of their peers on a daily basis. Subsequent changes in the students' energy consumption behaviours were analysed, and correlated with their cultural background, which was assessed using a survey instrument designed based on Hofstede's cultural dimensions model. The experiment results showed that the mean and variance of changes in energy consumption, in response to the provision of eco-feedback information, differed significantly between participants from different countries. The results also showed that all cultural dimensions were statistically correlated to the effectiveness of the eco-feedback system, which explained how different aspects of culture could influence the energy consumption behaviours of building occupants. The results suggested that eco-feedback technologies should be tailored to specific cultural context to improve their effectiveness in building energy conservation.

18/00630 Energy optimization for maximum energy saving with optimal modification in continuous catalytic regeneration reformer process

Babaqi, B. S. *et al. Energy*, 2017, 120, 774–784.

The heat integration retrofit analysis of the continuous catalytic regeneration reformer process (CCRRP) was conducted to determine the major opportunities for maximum energy saving via optimal modifications of the process design. Process data used from a real existing CCRRP were extracted, which are applicable in the pinch analysis technique (PAT). The present investigations of analysis showed a great opportunity for reducing energy consumption and costs at an optimum minimum approach temperature of 40 °F. Retrofit analysis of current process to achieve the optimal modifications of process included three additional heat exchangers with shells tube of two heat exchangers according to reduction in ΔT_{min} from 87 to 40 °F. The evaluation of maximum energy savings as new design indicated the reduction of utilities by about 32%, which led to reduce of the total cost index in the process of approximately 4.5%.

18/00631 Energy quality factor of materials conversion and energy quality reference system

Zheng, D. *et al. Applied Energy*, 2017, 185, 768–778.

This paper aims to explore the standardized data system of the exergy function and energy quality analysis methods. The concepts of the energy grades of the material and process were proposed. These concepts indicate that the availability factor is the thermodynamic property of the process, whereas the energy quality factor is the thermodynamic property of the substance. By evaluating the difference in the energy quality factors between different substances in material conversion processes, the energy-exchange mechanisms and the features of energy grade of processes can be revealed. The reference substance system was created by defining 100 kPa and 298.15 K as the pressure and temperature of environmental reference state and choosing air with an appropriate composition derived from the US Standard Atmosphere 1976 as the reference substance for atmospheric elements, pure water as the reference substance for hydrogen, and the pure compounds in the geosphere as the reference substance for other elements. Thus, a new energy quality reference state system, which involves fundamental models, the reference substances system, and data about the standard exergy and standard enthalpy of 81 elements, was established. In order to show how the new proposals could be used for the real applications, the energy cascade utilizations of the thermodynamic mechanisms of four CO_2-hydrogenation processes were analysed to evaluate CO_2 resource utilization routes, among which the CO and methanol routes are potential options.

18/00632 Energy saving potential of a two-pipe system for simultaneous heating and cooling of office buildings

Maccarini, A. *et al. Energy and Buildings*, 2017, 134, 234–247.

This paper analyses the performance of a novel two-pipe system that operates one water loop to simultaneously provide space heating and cooling with a water supply temperature of around 22 °C. To analyse the energy performance of the system, a simulation-based research was conducted. The two-pipe system was modelled using the equation-based Modelica modelling language in Dymola. A typical office building model was considered as the case study. Simulations were run for two construction sets of the building envelope and two conditions related to inter-zone air flows. To calculate energy savings, a conventional four-pipe system was modelled and used for comparison. The conventional system presented two separated water loops for heating and cooling with supply temperatures of 45 and 14 °C, respectively. Simulation results showed that the two-pipe system was able to use less energy than the four-pipe system thanks to three effects: useful heat transfer from warm to cold zones, higher free cooling potential and higher efficiency of the heat pump. In particular, the two-pipe system used approximately between 12% and 18% less total annual primary energy than the four-pipe system, depending on the simulation case considered.

18/00633 Estimating the potential for electricity savings in households

Boogen, N. *Energy Economics*, 2017, 63, 288–300.

Improving efficiency in the use of energy is an important goal for many nations since end-use energy efficiency can help to reduce CO_2 emissions. Furthermore, since the residential sector in industrialized countries requires around one third of the end-use electricity, it is important for policy makers to estimate the scope for electricity saving in households to reduce electricity consumption by using appropriate steering mechanisms. The level of technical efficiency in the use of electricity was estimated using data from a Swiss household survey. An average inefficiency in electricity use by Swiss households of around 20–25% was found. Bottom-up economic-engineering models estimate the potential in Switzerland to be around 15%. In this paper a sub-vector input distance frontier function based on economic foundations was used. The authors' estimates lie at the upper end of the electricity saving potential estimated by the afore-mentioned economic-engineering approach.

18/00634 Fossil energy saving and CO_2 emissions reduction performance, and dynamic change in performance considering renewable energy input

Chen, W. and Geng, W. *Energy*, 2017, 120, 283–292.

Energy environmental and non-radial Malmquist indexes are proposed employing a non-radial directional distance function to evaluate fossil energy saving and CO_2 emissions reduction performance, and dynamic change in performance internationally. Renewable energy is also proposed as an essential energy input for the models. An empirical study of 26 Organization for Economic Cooperation and Development countries and Brazil, Russia, India and China was performed, with the following outcomes: fossil energy saving and CO_2 emissions reduction performance is underestimated for most countries, regardless of renewable energy input, however, this underestimation has little influence on performance rankings; there is no significant correlation between the proportion of renewable energy consumption and fossil energy saving and CO_2 emissions reduction performance; the 30 countries can be divided into four categories with corresponding specific strategies for energy saving and emissions reduction; Generally, technological progress and efficiency improvement are out of sync, mainly because of the difficulty to achieve the efficiency improvements.

18/00635 Housing-related lifestyle and energy saving: a multi-level approach

Thøgersen, J. *Energy Policy*, 2017, 102, 73–87.

A new instrument for measuring housing-related lifestyle (HRL) is introduced and employed for identifying national and cross-national HRL segments in 10 European countries ($N = 3190$). The identified HRL segments are profiled and the practical importance of HRL for everyday energy-saving efforts in the home and for the energy-consumer's openness to new energy saving opportunities (i.e. energy saving innovativeness) is investigated. The HRL instrument's 71 items load on 16 dimensions within five lifestyle elements. Multi-group confirmatory factor analysis reveals that the instrument possesses metric but not scalar (measurement) invariance across the 10 countries. Multilevel latent class analysis is used to classify participants to HRL segments and the 10 countries into regions with similar segment structure. The optimal solution has seven HRL segments and three country classes, which are profiled in terms of relevant background characteristics. A multivariate GLM analysis reveals that when differences in housing-related lifestyles are controlled, neither country of residence nor the interaction between lifestyle and country of residence influence energy saving innovativeness or everyday energy-

saving efforts. However, these two behavioural tendencies vary significantly and substantially between lifestyle segments. The study shows that HRL segmentation is a useful tool for creating more targeted and effective energy-saving campaigns.

18/00636 Numerical assessment and optimization of a low-energy residential building for Mediterranean and Saharan climates using a pilot project in Algeria
Ali-Toudert, F. and Weidhaus, J. *Renewable Energy*, 2017, 101, 327–346.
The awareness for energy efficiency in buildings increasingly expands in Algeria, where a legal framework exists for promoting the utilization of regenerative energies. However, models of best practice are still relatively few. As a contribution, this paper reports on a study, which aims at finding out the best design strategies for affordable energy efficient residential buildings. The focus is put on the Mediterranean Algiers and the Saharan Ghardaia. Dynamic energy modelling was carried out using TRNSYS 17 to assess a residential house built as a MED-ENEC pilot project. The simulation is executed at two sequential stages: the reconnaissance stage where the building is compared to a typically non-insulated conventional construction and then the assessment stage, in which the pilot project already designed to low energy standards is investigated in an attempt to increase its energy efficiency further. By means of a parametric study, the most efficient passive design measures for minimizing heating and cooling energy demands were delineated and their dimensioning fixed. The results confirm (i) the easiness to save energy in comparison to the local inappropriate conventional building type, and (ii) possible additional energy savings in the pilot project, so that almost no heating is required and the cooling visibly further reduced.

18/00637 Potential life cycle energy savings through a transition from typical to energy plus households: a case study from Thailand
Iqbal, M. I. *et al. Energy and Buildings*, 2017, 134, 295–305.
Through a comparative life cycle analysis of typical, nearly net zero, net zero and energy plus houses in Thailand, each having a net floor area of 141.4 m^2; this study demonstrates that the operational electricity demand of typical houses can be reduced by 37% by incorporating various energy saving measures and goes further to establish that this reduced demand can be partially, fully or-over met through in-house electricity generation by solar photovoltaic. Over a period of 50 years, the transition from typical to nearly net zero and net zero energy houses is assessed to offer total life cycle primary energy savings of about 69% and 86%, respectively; while the energy plus house is assessed to have (i) a potential of feeding in 7450 kWh of electricity into the public grid each year and (ii) the capability of being energy neutral in a life cycle perspective over a duration of 16 years. The embodied energies through the evolution from typical to energy plus houses are however noted to grow up to 214%, mainly because of the manufacture of photovoltaic panels.

18/00638 Scenario analysis of energy saving and CO_2 emissions reduction potentials to ratchet up Japanese mitigation target in 2030 in the residential sector
Wakiyama, T. and Kuramochi, T. *Energy Policy*, 2017, 103, 1–15.
This paper assesses to what extent CO_2 emissions from electricity in the residential sector can be further reduced in Japan beyond its post-2020 mitigation target [known as 'intended nationally determined contribution' (INDC)]. The paper examines the reduction potential of electricity demand and CO_2 emissions in the residential sector by conducting a scenario analysis. Electricity consumption scenarios are set up using a time-series regression model, and used to forecast the electricity consumption patterns to 2030. The scenario analysis also includes scenarios that reduce electricity consumption through enhanced energy efficiency and energy saving measures. The obtained results show that Japan can reduce electricity consumption and CO_2 emissions in the residential sector in 2030 more than the Japanese post-2020 mitigation target indicates. At the maximum, the electricity consumption could be reduced by 35 TWh, which contributes to 55.4 $MtCO_2$ of emissions reduction in 2030 compared to 2013 if the voluntarily targeted CO_2 intensity of electricity is achieved. The result implies that Japan has the potential to ratchet up post-2020 mitigation targets discussed under the Paris Agreement of the United Nations Framework Convention on Climate Change.

18/00639 Sequential early-design guidance for residential single-family buildings using a probabilistic metamodel of energy consumption
Hester, J. *et al. Energy and Buildings*, 2017, 134, 202–211.
In order to reduce the energy consumption of a proposed building, it is valuable to be able to estimate the energy consumption at early stages of the design process when influential attributes are being decided upon. This study presents a novel use of a regression-based energy metamodel to guide the early design of single-family residential buildings by providing guidance on key early-design decisions through quantitative, probabilistic analyses that accommodate the flexibility and low detail of conceptual designs. Monte Carlo simulations provide a distribution of energy consumption predictions reflecting the design uncertainty, and sensitivity analyses reveal which parameters contribute the most to the variability in the metamodel output based on the current level of detail in the design. By sequentially specifying the most influential parameters, the authors show that the variability in predicted energy consumption can be reduced by approximately 90% (as measured by the coefficient of variation), even when the average input specification increases by only 40% compared to the original parameter ranges. A case study demonstrates that a statistically significant difference between design alternatives can be seen even when limited information is available for many aspects of the design.

17 ENERGY CONVERSION AND RECYCLING

18/00640 Analysis of the backpressure effect of an organic Rankine cycle (ORC) evaporator on the exhaust line of a turbocharged heavy duty diesel power generator for marine applications
Michos, C. N. *et al. Energy Conversion and Management*, 2017, 132, 347–360.
In marine and power generation sectors, waste heat recovery technologies are attracting growing attention in order to increase heavy duty diesel engines efficiency and decrease fuel consumption, with the purpose of respecting stringent emissions legislations. In this work, the backpressure effect of an organic Rankine cycle (ORC) evaporator on the exhaust line of a turbocharged, V12 heavy duty diesel engine, for typical marine and power generation applications has been investigated using the commercial software Ricardo WAVE. Three different state-of-the art turbocharging strategies are assessed in order to counterbalance the increased pumping losses of the engine due to the boiler installation: fixed turbine, waste-gate (WG) and variable geometry turbine (VGT). At the same time, the steady-state thermodynamic performance of two different ORC configurations, simple tail-pipe evaporator and recuperated simple tail-pipe evaporator layouts, are assessed, with the scope of further increasing the engine power output, recovering unutilized exhaust gas heat. Several different working fluids, suitable for medium-high temperature waste heat recovery, are evaluated and screened, considering, as well, health and safety issues. Thermodynamic cycle parameters such as, for example, evaporation and condensing pressures, working fluid mass flow and cycle temperatures, are optimized in order to obtain the maximum improvement in brake specific fuel consumption. From the engine side point of view, a VGT turbocharger is the most favourable solution to withstand increased backpressure, while, regarding the ORC side, between the considered fluids and layouts, acetone and a recuperated cycle show the most promising performance.

18/00641 Could spent nuclear fuel be considered as a non-conventional mine of critical raw materials?
Bourg, S. and Poinssot, C. *Progress in Nuclear Energy*, 2017, 94, 222–228.
Each year, more than 10,000 tons of spent fuels are discharged from nuclear power plants in the world. Heavy element nuclear fission reactions, at the origin of energy production, generate fission products of intermediary mass, some of them being considered nowadays as critical raw materials. The potential interest to treat these spent fuels in order to recycle these elements has risen recently following increasing international tensions on their supply for industry and energy. A study was carried out on the basis of the French nuclear fuel cycle scenario in order first to evaluate the inventory of such metals in spent fuel. The only elements of interest, since in significant amount, would be rare earth elements (REE) and platinum group metals (PGM). However, compare to the annual need of REE, the amount that would be recovered from spent fuels represent less than 0.01% of the annual world production. Because of the low price of these elements, there is no economic interest for such a recovery. The case of PGM, and specifically ruthenium and rhodium, is quite different. Even if a lower amount of these elements are in spent fuel, it represents 22% for Ru and 3.5% for Rh of the annual world production. The drawback is that these elements have numerous radioactive isotopes that forbid using them for industrial applications. 20–50 years of storage after separation would be necessary for ruthenium and rhodium to get a radioactivity level lower than potential clearance levels. Before any industrial use, very efficient separation processes would be required to selectively recover these elements. The physico-chemical forms of these elements

in the spent fuel make the work tricky. Finally, such a use would require the official existence of a clearance level for nuclear materials as recommended by the IAEA.

18/00642 Effect of fly ash on properties of crushed brick and reclaimed asphalt in pavement base/subbase applications

Mohammadinia, A. *et al. Journal of Hazardous Materials*, 2017, 321, 547–556.

Fly ash (FA), an abundant by-product with no carbon footprint, is a potential stabilizer for enhancing the physical and geotechnical properties of pavement aggregates. In this research, FA was used in different ratios to stabilize crushed brick (CB) and reclaimed asphalt pavement (RAP) for pavement base/subbase applications. The FA stabilization of CB and RAP was targeted to improve the strength and durability of these recycled materials for pavement base/subbase applications. The unconfined compressive strength (UCS) and resilient modulus (M_R) development of the stabilized CB and RAP aggregates was studied under room temperature and at an elevated temperatures of 40 °C, and results compared with unbound CB and RAP. Analysis of atomic silica content showed that when the amount of silica and alumina crystalline was increased, the soil structure matrix deteriorated, resulting in strength reduction. The results of UCS and M_R testing of FA stabilized CB and RAP aggregates indicated that FA was a viable binder for the stabilization of recycled CB and RAP. CB and RAP stabilized with 15% FA showed the highest UCS results at both room temperature and at 40 °C. Higher temperature curing was also found to result in higher strengths.

18/00643 Evaluation of waste materials for acid mine drainage remediation

Jones, S. N. and Cetin, B. *Fuel*, 2017, 188, 294–309.

Laboratory-scale tests were conducted to assess the efficiency of two different types of waste materials to remediate acid mine drainage (AMD). The waste materials used in the current study were recycled concrete aggregates (RCAs), and fly ashes. Four different RCA materials and three different fly ash materials were evaluated. Column leach tests (CLTs) were conducted to determine the effects of the remediation materials on pH, electrical conductivity, alkalinity, oxidation reduction potential (Eh), and concentrations of sulfate (SO_4^{2-}), chromium (Cr), iron (Fe), manganese (Mn), copper (Cu), and zinc (Zn) in AMD. Results of the CLTs suggest RCAs and one of the highly alkaline fly ash can effectively raise pH of the AMD and reduce concentrations of Cr, Cu, Fe, Mn, and Zn in AMD. In addition, sulfate concentrations of AMD decreased significantly after being treated by RCAs while sulfate concentrations of the AMD increased when it was remediated by fly ashes. It is speculated that leaching of sulfate from fly ash samples during treatment may decrease the metal sorption capacity of fly ashes. X-ray fluorescence spectroscopy quantified the impact of CaO and loos on ignition (LOI) in the remediation materials on sorption capacity of metals from the AMD. Sorption capacity for Cr, Cu, Fe, and Zn was found to be greater in materials with high CaO and LOI content, and low unburned carbon.

18/00644 Exploring the potential for waste heat recovery during metal casting with thermoelectric generators: on-site experiments and mathematical modeling

Børset, M. T. *et al. Energy*, 2017, 118, 865–875.

Thermoelectric power generators are scalable and simple systems for recovering waste-heat disposed by the industry. The authors combine on-site measurements and a mathematical model to study the potential for power generation with this technology from heat available from casting of silicon. They implement a 0.25 m^2 thermoelectric generator (TEG), based on bismuth-tellurium modules, in the casting area of a silicon plant. The measured peak power is 160 $W\,m^{-2}$ and the corresponding maximum temperature difference across the modules is 100 K. A large potential to increase the power generated beyond the measured values was predicted. For a two-fold increase of the heat transfer coefficient at the cold side, and by moving the generator closer to the heat source, it was predicted that the power output can reach 900 $W\,m^{-2}$. By tailoring the design of the TEG to the conditions encountered in the industrial facility, it is possible to generate more power with less thermoelectric material. The authors provide guidelines on how to design thermoelectric systems to maximize the power generation from waste heat given off from silicon during casting.

18/00645 Extraction and characterization of waste plastic oil (WPO) with the effect of *n*-butanol addition on the performance and emissions of a DI diesel engine fueled with WPO/diesel blends

Damodharan, D. *et al. Energy Conversion and Management*, 2017, 131, 117–126.

With growing global energy demands, recovering energy from waste plastic presents an attractive avenue to explore as it promotes recycling. Oil synthesized from waste plastic can be excellent fuel for diesel engines but yields higher carcinogenic smoke emissions and poor performance than fossil diesel (D). This study demonstrates the extraction and characterization of waste plastic oil (WPO) obtained by pyrolysis in a laboratory scale batch reactor and later sets out to investigate the effects of adding a renewable oxygenated component in the form of *n*-butanol (B), a naturally occurring biofuel. Three ternary blends, D50-WPO40-B10, D50-WPO30-B20 and D50-WCO20-B30 were strategically prepared to utilize both a recycled component (WPO by up to 40%) and a renewable component (*n*-butanol by up to 30%). The performance and emissions of DI diesel engine when fuelled with these blends was then analysed in comparison with both neat WPO and diesel operation. Results indicated that *n*-butanol addition presented lower smoke emissions and higher HC emissions when compared to diesel. Addition of 10% *n*-butanol by volume to WPO/ULSD blend reduced NO_x emissions favourably when compared to both WPO and diesel. However NO_x emissions were higher than the corresponding WPO case for higher volume *n*-butanol blends. Brake thermal efficiency (BTE) of the engine increased with increasing *n*-butanol fraction in the blends when compared to WPO. Fuel consumption of ternary blends was found to be better than WPO. D50-WPO40-B10 blend presented less NO_x and smoke emissions with improvement in engine performance when compared to diesel. Study revealed that *n*-butanol could be a viable additive for diesel engines operating with WPO extracted from mixed waste plastic.

18/00646 Microwave based oxidation process for recycling the off-specification $(U,Pu)O_2$ fuel pellets

Singh, G. *et al. Journal of Nuclear Materials*, 2017, 484, 81–90.

This paper reports development of a process named microwave direct oxidation (MWDO) for recycling the off-specification $(U,Pu)O_2$ mixed oxide (MOX) fuel pellets generated during fabrication of typical fast reactor fuels. MWDO is a two-stage, single-cycle process based on oxidative pulverization of pellets using 2450 MHz microwave. The powder sinterability was evaluated by bulk density and BET specific surface area. The oxidized powders were analysed for phases using XRD and stoichiometry by thermogravimetry. The sinterability was significantly enhanced by carrying out oxidation in higher oxygen partial pressure and by subjecting MOX to multiple micronization-oxidation cycles. After three cycles, the recycled powder from $(U,28\%Pu)O_2$ resulted surface area >3 m^2/g and 100% re-used for MOX fabrication. The flow sheet was developed for maximum utilization of recycled powder describable by a parameter called scrap recycling ratio (SRR). The process demonstrates smaller processing cycle, better powder properties and higher oxidative pulverization over conventional method.

18/00647 New ceramic materials from MSWI bottom ash obtained by an innovative microwave-assisted sintering process

Taurino, R. *et al. Journal of the European Ceramic Society*, 2017, 37, (1), 323–331.

Preliminary results on the production of new ceramic bricks by an innovative microwave-assisted sintering process employing MSWI bottom ashes are reported. Microwave heating technique was compared with a conventional thermal treatment with the aims to: (1) study the influence of heat treatment method on the crystallization behaviour and on the microstructure of obtained samples; (2) define the crystallization evolution in microwave field; (3) gain an insight into the physical properties of the new samples. Higher crystallinity and new crystal phases were observed in the samples prepared by microwave heating, where precipitation of new sodium rich crystal phases was observed, together with quartz and anorthite, formed in the conventionally prepared samples. The possibility to obtain novel bricks with huge waste amount, in a very short thermal cycle and at relatively low temperatures was demonstrated with significant reductions in the energy demand for their production. Finally, the samples obtained by microwave-assisted sintering are characterized by improved mechanical properties.

18/00648 Parametric study of a thermoelectric generator system for exhaust gas energy recovery in diesel road freight transportation

Vale, S. *et al. Energy Conversion and Management*, 2017, 133, 167–177.

A parametric study and optimization approaches of a thermoelectric generator (TEG) for the recovery of energy from the exhaust gas in diesel vehicles used in freight transport is reported. The TEG is installed in the tailpipe of a commercial vehicle (3.5 tonnes) and a heavy-duty vehicle (40 tonnes). The exhaust gas is used as the heat source and the cooling water as the heat sink. Two different heat exchanger configurations are considered: plain fins and offset strip fins. The influence of the height, length and spacing of the fins on the electrical and net power is analysed for the fixed width and length of the TEG. The influence of the length and width of the TEG and of the height of the thermocouple legs is also investigated. According to the criteria used in this study, plain fins are the best choice, yielding a

maximum electrical power of 188 W for the commercial vehicle and 886 W for the heavy-duty vehicle. The best recovery efficiency is about 2%, with an average thermoelectric material efficiency of approximately 4.4%, for the light-duty vehicle. Accordingly, there is significant room for further improvement and optimisation based on the thermoelectric modules and the system design.

18/00649 Pyrolysis of fibre residues with plastic contamination from a paper recycling mill: energy recoveries

Brown, L. J. *et al. Energy Conversion and Management*, 2017, 133, 110–117.

Pyrolysis is a promising technology for the production of marketable energy products from waste mixtures, as it decomposes heterogeneous material into homogenous fuel products. This research assessed the ability of slow pyrolysis to convert three waste streams, composed of fibre residues contaminated with different plastic mixtures, into char and tarry phase products at three different temperatures (300, 425 and 550 °C). The products were characterized in terms of mass yield, higher heating value (HHV) and gross energy conversion (EC). Significant amounts of hydrocarbon plastics in the feed materials increased the calorific values of the char (up to 32.9 MJ/kg) and tarry phase (up to 42.8 MJ/kg) products, comparable to high volatile bituminous A coal and diesel, respectively. For all three waste streams converted at 300 °C, the majority of the energy in the feedstock was recovered in the char product (>80%), while deoxygenation of fibre component resulted in char with increased calorific value (up to 31.6 MJ/kg) being produced. Pyrolysis at 425 °C for two of the waste streams containing significant amounts of plastic produced both a valuable char and tarry phase, which resulted in an EC greater than 74%. Full conversion of plastic at 550 °C increased the tarry phase yield but dramatically decreased the char HHV. The influence of temperature on product yield and HHV was discussed based on the pyrolysis mechanisms and in relation to the plastic composition of the waste streams.

18/00650 Supercritical CO_2 Rankine cycles for waste heat recovery from gas turbine

Kim, Y. M. *et al. Energy*, 2017, 118, 893–905.

A supercritical carbon dioxide (S-CO_2) Rankine cycle for waste heat recovery (WHR) from a gas turbine can achieve high efficiency despite its simplicity and compactness in comparison to a steam/water cycle. With respect to WHR, it is very important to maximize the net output power by incorporating the utilization efficiency of the waste heat in conjunction with the cycle thermal efficiency. A simple S-CO_2 Rankine cycle used for a high-temperature source cannot fully utilize the waste heat because the working fluid is preheated by the recuperator to a high temperature to achieve a high cycle efficiency. To recover the remaining waste heat from a simple cycle, a cascade cycle with a low-temperature (LT) loop can be added to the high-temperature (HT) loop, or a split cycle – in which the flow after the pump is split and preheated by the recuperator and LT heater separately, before the HT heater can be used. This study presents a comparison of three cycles in terms of energy and exergy analyses of their systems. The results show that a split cycle can produce the highest power of the threes systems considered over a wide range of operating conditions. The reasons for this are explained in detail.

18/00651 The production of hydrogen-rich gas by catalytic pyrolysis of biomass using waste heat from blast-furnace slag

Luo, S. *et al. Renewable Energy*, 2017, 101, 1030–1036.

The granulation for molten slag produces a large amount of sensible and recoverable heat. In this paper, a system was proposed to simultaneously produce glassy slag and reuse the heat for production of hydrogen-rich gas via biomass catalytic pyrolysis. A variety of parameters, including slag temperature, mass ratio of slag to biomass (S/B), particles size, and rotor speed, were evaluated for their effects on pyrolysis product yields and gas characteristics. The catalytic activity of blast-furnace (BF) slag for improving tar cracking was also addressed. The conditions of 1000 °C of slag temperature and 0.6 of S/B achieved a complete pyrolysis of biomass. When the S/B value increased to 0.8, a lower slag temperature (700 °C) can afford a complete pyrolysis of biomass. The maximum gas yield was gained at a rotor speed of 16 rpm/min, when slag particles in reactor showed a 'cascading' movement. BF slag exhibited a catalytic activity in tar cracking and C_nH_m reforming during biomass pyrolysis process. Furthermore, decreasing the slag particle size favoured to produce more light gases, and less char and condensate. However, the effect of slag particle size became not evident in the subsequent catalytic reforming process.

18/00652 Waste cooking oil-to-energy under incomplete information: identifying policy options through an evolutionary game

Zhang, H. *et al. Applied Energy*, 2017, 185, 547–555.

The policies concerning waste cooking oil-to-energy supply chains are urgently needed in China. This is because, in practice, there is a real risk of raw material supply being interrupted. Given that the various participating entities are often unable to accurately estimate either their own revenue stream or costs, or the actions of other stakeholders, this paper builds an evolutionary game to model three parties including the government, biofuel enterprises and restaurants under the assumptions of incomplete information and bounded entity rationality, and investigates supply chain policy options. Results indicate that the strategy choices of the various parties (dominance, treatment and participation) are merely in equilibrium for the time being. In the long run, however, there will be one of two equilibrium states: either all three players withdraw from supply chain operation or biofuel enterprises and restaurants eventually take an active part in reverse supply chain management without government intervention. To attain this long-term goal, governments should eliminate the garbage disposal fees levied on restaurants, while, at the same time, increase quantity-based subsidies to biofuel enterprises. Cracking down on restaurants that privately sell waste cooking oil to illegal peddlers should be regarded as a long-term task. Therefore, in either equilibrium state, restaurants should always be the focus of attention.