01 SOLID FUELS

Sources, winning, properties

17/01680 Characterization of coal blends for effective utilization in thermal power plants

Raaj, S. S. *et al. Applied Thermal Engineering*, 2016, 102, 9–16.

This paper deals with the characterization of coal blends using various conventional and advanced analytical techniques. There has been an increasing trend in utilizing imported coals for power generation in India and utilities are resorting to blended coal firing for various reasons, both financially as well as technically. Characterization studies were carried out on two combinations of Indian and imported coal blends. Conventional characterization such as proximate and ultimate analysis and determination of calorific value were carried out for the raw coals and blends as per ASTM standards. Following this thermal and mineral analysis of the samples were carried out using thermo-gravimetric analyser, X-ray fluorescence spectrometer and computer controlled scanning electron microscope. Combustion experiments were also conducted using drop tube furnace to determine the burnout of the raw coals and blends. The selection of technically suitable coal combination for blending, based on these characterization studies, has been detailed.

17/01681 Experimental study on ignition behavior of pulverized coal particle clouds in a turbulent jet

Xu, K. *et al. Fuel*, 2016, 167, 218–225.

Ignition behaviours of pulverized coal particle clouds in a jet with different turbulent intensity, O_2 concentration and coal concentration were experimentally studied using an entrained flow reactor. Mie scattering technique and high-speed cameras were employed to record the particle motions and flame behaviour. Results revealed that a cloud flame consisted of a number of parcel flames and stripe flames, which were located in the centre and around boundary of the cloud flame, and resulted by the burning of the evolved volatile matter or the clusters of fine fuel particles, and the burning of the single particles respectively. As Reynolds number of the primary flow increased, the cloud flame changed from narrow and structured to wide and turbulent. At the same time, the particle dispersion became more intensive, leading to a lower flame incandescence. The increase of O_2 concentration in the primary or secondary flow promoted ignition of cloud flames. For laminar cloud flame, ignition distance was more sensitive the O_2 concentration in the primary flow, and a minimum value was found at certain coal concentration, but for turbulent cloud flame, ignition distance was shorter, and no obvious non-monotonic trend was found over the tested coal concentration range.

Preparation

17/01682 Converting lignite to caking coal via hydro-modification in a subcritical water–CO system

Zhao, Y. *et al. Fuel*, 2016, 167, 1–8.

The conversion of lignite to caking coal via hydro-modification was conducted in a subcritical water–CO system, and the effects of the hydro-modification on the coal structure were investigated by Soxhlet extraction, thermogravimetry, Fourier transform infrared spectroscopy and electron spin resonance. The results indicate that the caking property of lignite can be clearly developed and that the caking index (G_{RI}) of modified coal increases from 0 to 96. The active hydrogen ($H^{\cdot}$) produced from the water gas shift reaction (WGSR) provides an important hydrogen source for the hydro-modification of coal, and the G_{RI} strongly depends on the variation of CO conversion (X_{CO}). The optimum G_{RI} is registered at X_{CO} values of 36.48–43.48%. The cleavage of bridge-bonds and side-chains improves the mobility of molecules in lignite, which promotes the rearrangement of aromatic lamellar to generate polyaromatic free radicals that could be stabilized by $H^{\cdot}$ to form plastic species. The moderate decomposition of lignite and the appropriate amount of active hydrogen ($H^{\cdot}$) favour an increase in the extraction yield of preasphaltene, which correlates well with the caking index (G_{RI}), allowing for the development of a plastic stage the modified coals.

17/01683 Pyrolysis of lignite following low temperature ionic liquid pretreatment

Lei, Z. *et al. Fuel*, 2016, 166, 124–129.

A new and effective method, lignite pyrolysis with pretreatment with ionic liquid 1-butyl-3-methyl-imidazolium chloride ([Bmim]Cl) at low temperature, was studied. It is found that [Bmim]Cl pretreatment increased the total yield of liquid products and oil fractions compared to original lignite. The pretreatment temperature and the ratio of [Bmim]Cl to lignite play key roles on the increase of total liquid yield and the change of tar composition. The increases of liquid products yield and oil fractions content are found to be caused by the changes of composition of oxygen-containing functional groups in lignite through [Bmim]Cl pretreatment. It is also found that [Bmim]Cl can be efficiently recovered and the pretreatment performance of regenerated [Bmim]Cl is slightly lower than that of fresh [Bmim]Cl.

17/01684 The exergy release mechanism and exergy analysis for coal oxidation in supercritical water atmosphere and a power generation system based on the new technology

Yan, O. *et al. Energy Conversion and Management*, 2016, 129, 122–130.

The oxidation environment has important influence on the transformation of the energy contained in fuel and generation of pollutants. To the problem of nearly 50% exergy losses in coal oxidation at air atmosphere, this research intends to change oxidation atmosphere from air to supercritical water/oxidant and achieve efficient release of exergy in coal at about 650 °C with the aid of a high solubility and unique performance of heat and mass transfer of supercritical water. Therefore, firstly, based on the exergy analysis theory and the energy-utilization diagrams, the release mechanism of exergy of coal in supercritical water oxidation process is revealed. It is pointed out that supercritical water oxidation has changed the release pathways of chemical exergy, and decreased the level difference between chemical exergy and thermal energy, and more exergy is released. Meanwhile, there is also no exergy loss of physical heat transfer. As a result, supercritical water oxidation has higher exergy efficiency than conventional oxidation. Secondly, the exergy losses, level difference between chemical exergy and thermal energy as well as exergy efficiency, are quantitatively investigated. Results show that the exergy efficiency of supercritical water oxidation reactor may be as high as 80.1% and has increased by 27% relative to conventional boilers. Thirdly, based on supercritical water oxidation of coal, a concept power generation system is constructed. Exergy efficiency is calculated and exergy analysis is provided for the supercritical water oxidation power plant. Compared with conventional power plant, exergy efficiency in supercritical water oxidation plant reaches as high as 61.3% and 21% higher than that in conventional power plant. Finally, from the results obtained, it is believed that the commercial breakthrough of the supercritical water oxidation process will be possible when the corrosion and salt deposition in the reactor are solved.

Economics, business, marketing, policy

17/01685 Assessing market structures in resource markets – an empirical analysis of the market for metallurgical coal using various equilibrium models

Lorenczik, S. and Panke, T. *Energy Economics*, 2016, 59, 179–187.

The prevalent market structures found in many resource markets consist of high concentration on the supply side and low demand elasticity. Market results are therefore frequently assumed to be an outcome of strategic interaction between producers. Common models to investigate the market outcomes and underlying market structures are games representing competitive markets, strategic Cournot competition and Stackelberg structures that take into account a dominant player acting first followed by one or more players. The authors add to the literature by expanding the application of mathematical models and applying an equilibrium problem with equilibrium constraints (EPEC), which is used to model multi-leader–follower games, to a spatial market. Using their model, the authors investigate the prevalent market setting in the international market for metallurgical coal between 2008 and 2010, whose market characteristics provide arguments for a wide variety of market structures. Using different statistical measures to compare model results with actual market outcomes, it was found that two previously neglected settings perform best: first, a setting in which the four largest metallurgical coal exporting firms compete against each other as Stackelberg leaders, while the remainders act as Cournot followers, and second, a setting with BHP Billiton acting as sole Stackelberg leader.

17/01686 Estimating impact of regional greenhouse gas initiative on coal to gas switching using synthetic control methods

Kim, M.-K. and Kim, T. *Energy Economics*, 2016, 59, 328–335.

Fuel switching from coal to much cleaner natural gas in electricity generation is one of significant factors explaining the recent substantial reduction in greenhouse gas emissions in the Regional Greenhouse Gas Initiative (RGGI) region (north-eastern USA). Coal-to-gas switching has been triggered by the recent shale gas revolution, which the entire USA has experienced, not the RGGI region alone. If RGGI as a cap-and-trade carbon program did not work effectively, the rate of fuel switching would have been similar to that of other US states. To estimate the effects of RGGI implementation in terms of the fuel switching, the synthetic control method was used for comparative case studies. The results provide strong evidence that coal-to-gas switching has been actually accelerated by RGGI implementation. RGGI increases gas share in electricity generation in the RGGI region by roughly 10–15% point higher than the synthetic RGGI.

17/01687 How energy technology innovation affects transition of coal resource-based economy in China

Guo, P. *et al. Energy Policy*, 2016, 92, 1–6.

The aim of this research paper is to investigate factors and mechanisms that may facilitate the transition from coal resource-based economy to sustainability. Based on the energy technology innovation theory, factors that may influence the transition of coal resource-based economy were categorized into four types, including: innovation policy, innovation input, innovation ability, and innovation organization. Hypotheses were proposed regarding the mechanisms of these factors. Data were collected from surveys administered to 314 Chinese energy firms, and a structural equation model (SEM) was employed to test the hypotheses. Ten of 15 hypotheses were retained based on the reliability tests, validity tests, and SEM. The results show that the four proposed factors are crucial in transforming the coal resource-based economy, and the effects become statistically significant through three intermediate variables, namely, transition of energy consumption structure, correction of resource wealth investment, and improvement of transition environment.

17/01688 Optimal extraction policy when the environmental and social costs of the opencast coal mining activity are internalized: mining District of the Department of El Cesar (Colombia) case study

Perdomo Calvo, J. A. and Jaramillo Pérez, A. M. *Energy Economics*, 2016, 59, 159–166.

Several articles have confirmed the social and environmental consequences of opencast coal mining. The main purpose of this study is to simulate the optimal extraction policy of coal mining with and without the internalization of the environmental and social monetary costs that occur in the mining district (located in the central part of the Department of El Cesar in Colombia) using discrete dynamic programming (backward recursion, discrete state Markov decision model and Bellman equation). Results indicate that the private optimal of the overproduction policy for the terminal phase of the resource extraction programme can be reduced once the negative externalities produced by mining practices are internalized into the cost function of the mining investment companies in Colombia. This means that if there is an increase in the total cost of extraction to offset the environmental and social impacts generated, the negative externalities would be less than or equal to the current level. Likewise, profits would continue being positive for the mining firms at the mining district.

Derived solid fuels

17/01689 An enhanced anaerobic membrane bioreactor treating bamboo industry wastewater by bamboo charcoal addition: performance and microbial community analysis

Xia, T. *et al. Bioresource Technology*, 2016, 220, 26–33.

In this study, two anaerobic membrane bioreactors (AnMBRs) were operated for 150 days to treat bamboo industry wastewater (BIWW), and one of them was enhanced with bamboo charcoal (BC, B-AnMBR). During the steady period, average chemical oxygen demand (COD) removal efficiencies of $94.5 \pm 2.9\%$ and $89.1 \pm 3.1\%$ were achieved in B-AnMBR and AnMBR, respectively. The addition of bamboo charcoal (BC) increased the amount of biomass and improved the performance of the systems. A higher biogas production and methane yield were also observed in B-AnMBR. Regarding the issue of membrane fouling, BC lowered the soluble microbial product (SMP) content by approximately 62.73 mg/L and decreased the membrane resistance, thereby mitigating membrane fouling. Analysis of the microbial communities demonstrated that BC increased the microbial diversity and promoted the activity of *Methanosaeta*, *Methanospirillum* and *Methanobacterium*, which are dominant in methane production.

17/01690 An optimized regulating method for composting phosphorus fractions transformation based on biochar addition and phosphate-solubilizing bacteria inoculation

Wei, Y. *et al. Bioresource Technology*, 2016, 221, 139–146.

The study was conducted to investigate the influence of biochar and/or phosphate-solubilizing bacteria (PSB) inoculants on microbial biomass, bacterial community composition and phosphorus (P) fractions during kitchen waste composting amended with rock phosphate (RP). There were distinct differences in the physico-chemical parameters, the proportion of P fractions and bacterial diversity in different treatments. The contribution of available P fractions increased during composting especially in the treatment with the addition of PSB and biochar. Redundancy analysis showed that bacterial compositions were significantly influenced by P content, inoculation and biochar. Variance partitioning further showed that synergy of inoculated PSB and indigenous bacterial communities and the joint effect between biochar and bacteria explained the largest two proportion of the variation in P fractions. Therefore, the combined application of PSB and biochar to improve the inoculation effect and an optimized regulating method were suggested based on the distribution of P fractions.

17/01691 Cokes of different origin as precursors of graphene oxide

Sierra, U. *et al. Fuel*, 2016, 166, 400–403.

This study demonstrates that pregraphitic materials (cokes) of different origin (petroleum and coal derivatives) can be used as precursors of graphene oxides. Two carbochemical cokes and a petrochemical one were oxidized and the resultant coke oxides exfoliated by ultrasounds to yield the corresponding graphene oxide materials. These were characterized in terms of the lateral size of the sheets, morphology and chemical composition. The new generation of graphene oxides prepared with coke exhibits similar characteristics to those traditionally obtained from graphite. It is also established that as larger the crystalline structure of the coke is, the higher the graphene oxide yields and the larger the size of the sheets.

17/01692 Computational homogenization in RVE models with material periodic conditions for CNT polymer composites

Song, W. *et al. Composite Structures*, 2016, 137, 9–17.

Representative volume element (RVE) models with material periodic conditions are developed in generating a three-dimensional (3D) network of fillers within the RVE. Computational homogenization in 3D RVE models is achieved using two approaches. In the first approach, statistical analysis with number of realizations is performed with increasing RVE size of randomly generated carbon nanotube (CNT) within polymer. In statistical analysis, the filler that exceeds the RVE are translated until they find new spatial location within RVE. Simulations with increasing RVE size are performed until the standard deviation of computed apparent property for each RVE size is minimum to predict the critical RVE size. In the second approach, RVE models with material periodic boundary conditions are developed, which involve placing fillers that exceed the RVE into their respective position on the opposite face of RVE as if the RVE is part of a larger network of RVEs. Percolation threshold analysis of CNT filled polymer composites is presented using both computational homogenization approaches. It is demonstrated that computational homogenized models with material periodic conditions are independent of RVE size and provide homogenized results and are computationally efficient compared to statistical models.

17/01693 Effects of steam and CO_2 on the characteristics of chars during devolatilization in oxy-steam combustion process

Xu, J. *et al. Applied Energy*, 2016, 182, 20–28.

Oxy-steam combustion is considered as one of promising technologies for the next generation oxy-fuel combustion, in which coal mainly burns in O_2/H_2O atmosphere. This work aims to investigate the devolatilization characteristics of coal in oxy-steam combustion and clarify the potential effects of steam and CO_2 on the char characteristics. Chars of a Chinese lignite were prepared in a fixed-bed reactor at 1050 °C under various steam/CO_2/N_2 atmospheres and characterized by a FT-IR/Raman spectrometer and thermogravimetric analyser. The results indicate the char yield during devolatilization in oxy-steam combustion was lower than that in N_2 atmosphere, and the steam gasification reaction played the key role. The high concentration of steam would significantly accelerate the condensation of aromatic rings in the char, and more condensed char would form during devolatilization in oxy-steam combustion compared to that in N_2 atmosphere. CO_2 in high concentration of steam had little effects on the char yields but it could participate in the cross-linking reactions on the char surface and partly reduce the condensation of the chars during devolatilization. Steam and CO_2 gasification reactions can not only speed up the consumption of the original O-containing functional groups in the coal but also bring some additional O-containing functional groups in the char. The

reactivity of the char formed during devolatilization in oxy-steam combustion was lower than that in N_2. A good linear relationship between the Raman band area ratio $I_{(Gr+Vl+Vr)}/I_D$ and char reactivity confirmed the decrease of the char reactivity was mainly attributed to the condensation of the char.

17/01694 Formation and decomposition of methane hydrate in coal

Smirnov, V. G. *et al. Fuel*, 2016, 166, 188–195.

The formation of methane hydrate from water adsorbed on the surface of natural bituminous coal has been studied. The state of the adsorbed water has been examined with DSC and NMR techniques. The isotherm of adsorption of water on coal has been studied. The experiments have shown that the water adsorbed on the coal studied is bound and non-freezing, i.e., no ice formation and melting occurs on cooling and heating of the coal samples containing the adsorbed water. This water undergoes a glass-like transition. The adsorbed water can be divided into strongly bound and weakly bound, in accordance to known models of water sorption by coals. Cooling and heating of containing adsorbed water coal samples under methane pressure results in expressed pressure anomalies corresponding to the formation and decomposition of the methane hydrate. Thus, the non-freezing water is capable of forming gas hydrate. It has been demonstrated that the hydrate is formed only from the weakly bound water. The equilibrium pressure and temperature parameters of this hydrate are identical to those of the bulk hydrate. Thus, it has been shown that at proper pressure and temperature gas hydrates can be formed in coals even in absence of free water. The results obtained make possible to suggest that the hydrophilic areas of the coal surface are active sites of gas hydrate nucleation.

17/01695 Kinetics of CO_2 and steam gasification of Victorian brown coal chars

Tanner, J. and Bhattacharya, S. *Chemical Engineering Journal*, 2016, 285, 331–340.

This work reports a kinetic study of the CO_2 and steam gasification of Victorian brown coal chars produced by rapid pyrolysis in a vertical drop tube furnace under entrained flow conditions. The study was performed by atmospheric pressure thermogravimetry over a temperature range of 650–1100 °C. The intrinsic kinetic parameters for the chemical rate control regime were determined, and the onset temperature of mass transfer limitations observed. The experimental results were well described by the volumetric model, grain model and random pore model for char conversion from 10% to 50% due to the high porosity created during rapid pyrolysis. Activation energies ranging from 162 to 175 kJ/mol and 119 to 165 kJ/mol were determined for CO_2 and steam gasification of Morwell, Loy Yang and Yallourn coal chars, respectively. The pre-exponential factors were of similar orders of magnitude, and increased for a smaller particle size range. The instantaneous relative reactivities, $k(H_2O)/k(CO_2)$, at 800 °C for the three Victorian brown coal chars ranged from 1.2 to 2.5, indicating a significant influence of the partial pressure of gasification reagent. The dominant influence in the case of CO_2 gasification reactivity of these chars appears to be similar for all three coals and is morphological in nature. The order of increasing activation energies for char-steam gasification correlated well with the molar ratio Na/(Ca + Na) in the char.

17/01696 Role of water and fine solids in onset of coke formation during bitumen cracking

Nhieu, P. *et al. Fuel*, 2016, 166, 152–156.

The aim of this study was to examine the effect of water and fine solids on coke formation during thermal cracking of a residue fraction from vacuum distillation (Athabasca vacuum tower bottoms) and Athabasca bitumen froth. Experiments were conducted in a batch reactor with 0–33.3 wt% water at 410 °C for up to 80 min to measure the time of onset of coke formation, total coke yield as a function of time, and conversion of vacuum residue. Removal of fine solids significantly shortened the onset time of coke formation, but the addition of water had no significant impact on onset time. The yield of cracked products, as determined by simulated distillation, was insensitive to the presence of water and fine solids. Based on the findings from this study, it was concluded that residual fine solids have a beneficial effect on thermal upgrading as they delayed the onset of coke formation, while water has little impact within the tested concentration range of 0–33 wt% water.

17/01697 Tailoring hierarchically porous graphene architecture by carbon nanotube to accelerate extracellular electron transfer of anodic biofilm in microbial fuel cells

Zou, L. *et al. Journal of Power Sources*, 2016, 328, 143–150.

To overcoming their respective shortcomings of graphene and carbon nanotube, a hierarchically porous multi-walled carbon nanotube@reduced graphene oxide (MWCNT@rGO) hybrid is fabricated through a versatile and scalable solvent method, in which the architecture is tailored by inserting MWCNTs as scaffolds into the rGO skeleton. An appropriate amount of inserted 1-D MWCNTs not only effectively prevent the aggregation of rGO sheets but also act as bridges to increase multidirectional connections between 2-D rGO sheets, resulting in a 3-D hierarchically porous structure with large surface area and excellent biocompatibility for rich bacterial biofilm and high electron transfer rate. The MWCNT@$rGO_{1:2}$/biofilm anode delivers a maximum power density of 789 mW m^{-2} in *Shewanella putrefaciens* CN32 microbial fuel cells, which is much higher than that of individual MWCNT and rGO, in particular, 6-folder higher than that of conventional carbon cloth. The great enhancement is ascribed to a synergistic effect of the integrated biofilm and hierarchically porous structure of MWCNT@$rGO_{1:2}$/biofilm anode, in which the biofilm provides a large amount of bacterial cells to raise the concentration of local electron shuttles for accelerating the direct electrochemistry on the 3-D hierarchically porous structured anodes.

17/01698 Thermochemical performance of carbon nanotubes based hybrid materials for $MgO/H_2O/Mg(OH)_2$ chemical heat pumps

Mastronardo, E. *et al. Applied Energy*, 2016, 181, 232–243.

Newly developed hybrid materials made of magnesium hydroxide and carbon nanotubes were proposed as heat storage medium for $MgO/H_2O/Mg(OH)_2$ chemical heat pumps. Samples were synthesized by deposition-precipitation method varying the $Mg(OH)_2$ load (32–52 wt%) and the type of carbon nanotubes, pristine or functionalized. The performances of the synthesized materials were evaluated by thermogravimetric analysis, which simulates the chemical heat pump cycle. The presence of the carbonaceous material positively affected the reaction performances, so that the hybrid materials showed improved heat storage/output capacity and faster heat output rate compared to pure $Mg(OH)_2$. The functionalization treatment and a proper $Mg(OH)_2$ load were fundamental to better the dispersibility of $Mg(OH)_2$ into the carbon nanotubes bundles which in turn enhanced the thermochemical performance of the active material, fully exploiting for the first time its maximum potential heat storage capacity, that is $\sim$1300 kJ/$kg_{Mg(OH)2}$, thus bringing the development of this technology to a level closer to its industrial application.

02 LIQUID FUELS

Sources, properties, recovery

17/01699 Alternative method for bulk modulus estimation of diesel fuels

Armas, O. *et al. Fuel*, 2016, 167, 199–207.

The knowledge of diesel fuel properties has great relevance for the analysis and comprehension of phenomena related to fuel injection, fuel–air mixture formation and diesel combustion processes. This work proposes an alternative method for estimating the bulk modulus of diesel fuels by means of an experimental installation commonly used for determining fuel injection rates from common rail injection systems. Three fuels were tested in the mentioned installation: commercial diesel fuel (blended with 5.8% of biodiesel), hydro-treated vegetal oil (HVO) and gas to liquid (GTL) fuel from natural gas by means of low temperature Fischer–Tropsch process. Results were obtained by testing two different injectors (solenoid operated and piezoelectric injectors) under different injection pressures and energizing times. Fuel temperature at inlet of the high pressure injection pump was controlled, keeping constant the pressure inside the fuel injection indicator. From the experimental work, data analysis and post-processing, bulk modulus of fuels tested has been estimated and compared to results obtained by diverse authors with different experimental installations and methods. Results obtained in this work show small differences compared to published data. Additionally, the initial time lag between the signal of the electric pulse when the injector is energized and the beginning of the injection rate profile depends only on the type of injector without influence of type of fuel and operating conditions. However, the rear time lag between both mentioned profiles depends only on injector type (when the solenoid operated injector was tested) while, with piezoelectric injector, it also depends on both energizing time of the injector and injection pressure.

17/01700 Catalytic combustion of methanol on Pt–Fecralloy foams prepared by electrodeposition

Cimino, S. *et al. Chemical Engineering Journal*, 2016, 285, 276–285.

The catalytic combustion of methanol in air under lean dry conditions has been studied using Pt–Fecralloy catalysts. These catalysts were prepared by cathodic electrodeposition of Pt onto commercial 50 ppi Fecralloy foams, controlling the noble metal loading through the Pt deposition charge. The catalysts were characterized by SEM and XRD at three different stages (as-prepared, after 2 h pretreatment at 600 °C in air and after use in methanol combustion) and their Pt surface area was estimated by cyclic voltammetry. In combustion tests, methanol oxidation started at temperatures as low as 80 °C, and reached 100% conversion to CO_2 at temperatures that decreased progressively for Pt loadings increasing from 0.8 to 13 mg cm^{-3}. The apparent activation energy of methanol combustion was estimated to be 68–70 kJ mol^{-1}, independent of the Pt loading of the samples. Repeated combustion cycles converged with SEM, XRD characterization of used catalysts to prove the stability of Pt–Fecralloy, under the conditions employed in the tests.

17/01701 Experimental study of fuel evaporation characteristics

Yan, Y. *et al. Fuel*, 2016, 169, 33–40.

Fuel evaporation characteristics are very important for the design of combustors. To quantitatively measure the fuel evaporation ratio of jet fuel in air cross flow, optical and physical measurement methods are proposed separately. The optical measurement method combines a high-speed camera and image-processing technologies, where as the physical measurement method applies the centrifugal force of a cyclone separator. The fuel evaporation ratio at different inlet conditions and different measurement cross-sections is analysed separately for jet fuel in air cross flow. Finally, the experimental results of the physical method are compared with those of the optical method. The experimental results show that (1) the results of the optical measurement method are in good agreement with those of the physical measurement method, and these two methods can be used to quantitatively measure the fuel evaporation ratio at individual test cross-sections; (2) when other inlet parameters are the same, the fuel evaporation ratio at the test cross-section gradually increases with increasing inlet air Weber number; (3) when other inlet parameters are the same, the fuel evaporation ratio at the test cross-section gradually decreases with increasing momentum ratio; and (4) when inlet parameters are the same, the fuel evaporation ratio at the test cross-section increases sharply with increasing distance between the test cross-section and nozzle.

17/01702 Gas hydrate plug formation in partially-dispersed water–oil systems

Akhfash, M. *et al. Chemical Engineering Science*, 2016, 140, 337–347.

The formation of gas hydrate plugs in deep water oil and gas flowlines poses severe operational and safety hazards. Previous work has established a mechanism able to describe plug formation in oil-continuous systems, which relies on the assumption that all the water remains emulsified in the oil phase. However, light hydrocarbon fluids, including condensates, may not stabilize water-in-oil emulsions, and the current mechanistic model cannot reliably assess the risk of plug formation in this scenario. This study presents a comprehensive set of experiments conducted in a high-pressure sapphire autoclave apparatus using 10–70 vol% water in partially-dispersing mineral oil at three fixed rotational speeds: 300, 500 and 900 rpm. Pressure and temperature were monitored continuously in the autoclave, providing direct estimates of hydrate growth rate, alongside measurements of the motor torque required to maintain constant mixing speed. A new conceptual mechanism for plug formation has been developed based on the visual observations made during these experiments, where a small hydrate fraction (2–6 vol%) in the oil phase was observed to disrupt the stratified water–oil interface and help disperse the water into the oil. This disruption was followed by an increase in the hydrate growth rate and particle agglomeration in the oil phase. In the final stages of hydrate growth for systems with low turbulence and high watercut, hydrate particles in the visual autoclave were observed to form a moving bed followed by full dispersion of water and oil, rapid hydrate growth and deposition on the wall. These rapid hydrate growth and deposition mechanisms significantly increased the maximum resistance-to-flow for partially-dispersing systems in comparison with mixtures that are fully dispersed under similar conditions.

Transport, refining, quality, storage

17/01703 Artificial neural networks for the analysis of spread mooring configurations for floating production systems

de Pina, A. A. *et al. Applied Ocean Research*, 2016, 59, 254–264.

This work presents the development of artificial neural networks for the analysis of any arbitrarily defined spread-mooring configuration for floating production systems, considering a given scenario characterized by the water depth, metocean data, characteristics of the platform hull, and the riser layout. The methodology is applied to recent designs of deepwater semi-submersible platforms connected to a large number of risers with asymmetrical layout. In such cases, the design variables may include values for the azimuthal spacing and mooring radius varying along the corners of the platform, besides the pretension and material of the lines. The results of the case study indicated that, given any mooring configuration characterized by the combination of all these design variables, the artificial neural networks provide fairly accurate values for the parameters of the response that are required for the design of mooring systems (typically platform offsets and line tensions).

17/01704 Catalytic cracking of heavy oil over TiO_2–ZrO_2 catalysts under superheated steam conditions

Kondoh, H. *et al. Fuel*, 2016, 167, 288–294.

Heavy oil upgrading was examined over titania–zirconia mixed oxide (TiO_2–ZrO_2) catalysts using fixed-bed flow-type reactors. Catalytic cracking of atmospheric residual oil (AR) and oil sand bitumen into lighter fuels such as gas oil and vacuum gas oil (VGO) was carried out in a superheated steam. The upgrading mechanisms were found to occur by carbon–carbon bond cleavage and naphthalene-ring opening caused by cracking, oxidation, or hydrogenolysis. The carbon–carbon bond cleavage reaction over acid sites is a well-known fluid catalytic cracker (FCC) process, whereas coke formation on catalysts is a serious problem. Hence, repetition of the sequence of reactions over a short period of time and immediate regeneration of the catalyst is required. The authors had previously developed a CeO_2–ZrO_2–Al_2O_3–FeO_X iron oxide catalyst for heavy oil conversion into lighter fuels (Funai *et al.* , 2010a,b; Kondoh *et al.* , 2015). When this catalyst was applied to the degradation of heavy oil, the lattice oxygen in the catalyst was the main active site, and it decomposed the heavy oil through partial oxidative cracking. Although the catalyst showed a high upgrading activity, it was gradually deactivated due to carbon deposition. In contrast, it was found that TiO_2–ZrO_2 catalysts exhibited acidic cracking activity for heavy oil cracking under superheated steam conditions. In this study, the authors conducted experiments with TiO_2–ZrO_2 catalysts for upgrading heavy oil. The effect of the catalyst composition on the yield of the lighter fuels, catalyst activity, and stability after the reaction was examined. As a result, the yield of light fractions from AR decomposition reached 71 mol%-C when using a TiO_2–ZrO_2 catalyst comprising TiO_2 and ZrO_2 in equimolar amounts and the catalyst structure remained intact after the reaction.

17/01705 Fatty acid methyl ester (FAME) composition used for estimation of biodiesel cetane number employing random forest and artificial neural networks: a new approach

Miraboutalebi, S. M. R. *et al. Fuel*, 2016, 166, 143–151.

Cetane number (CN) is the property used to evaluate the quality of biodiesels. The CN is mainly affected by the fatty acids methyl ester (FAME) composition of the biodiesel. The common experimental methods of determining CN are expensive, time consuming and are not always accurate, so it is vital to use other methods to predict CN. In this work, random forest (RF) and artificial neural networks (ANN) methods assisted by 10-fold cross-validation were employed to present appropriate, reliable and more generalized models for the prediction of CN based on experimental data of 131 different FAMEs collected from literature. Two different regression models were obtained based on these methods. The root mean squared error (RMSE) and the coefficient of determination (R^2) of 0.95, 2.53 for the ANN model, and 0.92, 3.09 for the RF model showed the high accuracy of these models. In term of accuracy, the ANN model showed better results compared to the RF model. On the other hand, in term of transparency and ease of interpretation, the RF model could be widely applied in CN determination. The positive effect of FAMEs on CN was obtained if stearic acid or myristic acid was higher than 51.95% or 44.95% regardless of other FAME acid percentages. In addition, values greater than 68.4% in linolenic acid could lead to a negative effect of that acid on CN.

17/01706 Modeling of kinetic-based catalyst grading for upgrading shale oil hydrogenation

Dai, F. *et al. Fuel*, 2016, 166, 19–23.

In this work, shale oil hydrogenation was upgraded in a two fixed-bed reactors to maximize light fraction with ultra-low sulfur and nitrogen. Three types of catalyst grading for shale oil hydroprotection, hydrofining, and hydrocracking were investigated to evaluate the hydrogenation performance. A lumping kinetic model of hydrodesulfurization, hydrodenitrification, and hydrocracking based on catalysts grading was established for the first time. Model parameters were determined using the Levenberg–Marquardt optimization algorithm. Results revealed that the model could accurately predict the removal

rations of sulfur, nitrogen, and desired product yields in shale oil hydrogenation under different catalyst grading. Thus, the model can be used for optimization of catalyst stacking to meet the requirements of hydrogenation products.

17/01707 Phospholipid transesterification in sub-/supercritical methanol with the presence of free fatty acids

Bi, Z. and He, B. B. *Fuel*, 2016, 166, 461–466.

Phospholipids and free fatty acids (FFA), along with triglycerides, are naturally formed constituents in unrefined vegetable oils and other plant lipids. Presence of phospholipids and FFA in such oils can cause processing difficulties, such as saponification and decrease in catalytic efficiency, thus lead to an adverse process efficiency in the transesterification of such oils for biodiesel production. This phenomenon was also observed in a previous study on converting microalgal lipids to fatty acid methyl esters (FAME) via *in situ* transesterification. This study aimed at further exploring the transesterification of phospholipids and investigating the effects of FFA presence and other processing conditions in biodiesel production from plant oils in sub- and/or supercritical methanol (SubCM/SCM). Experiments were carried out in a batch reactor in SubCM/SCM under various conditions without addition of catalysts. Pure chemicals of lecithin and stearic acid were used as the model compounds for phospholipids and FFA, respectively. The product yield (FAME in mol%) of the phospholipids after transesterification, as affected by the presence of FFA under different conditions, was selected as the respond factor to determine the process efficiency. Experimental results showed that phospholipids can be converted into FAME in such a process. Transesterification of phospholipids is largely affected by the interactive effect of operating temperature and reaction time. The increase in product yield is proportional to the increases in temperature and/or reaction time. The maximum product yield of 68.1 mol% was achieved at 250 °C and 120 min without the presence of FFA. The product yield started to level off once the system reached the SCM state. When temperature was held at 290 °C for 30 min, the product yield dropped to 33.6 mol%. Another phenomenon observed is that the presence of FFA enhances considerably the lipid conversion. The study revealed that phospholipids can be converted to FAME with a highest product yield of 93.9 mol% at 250 °C for 120 min in SCM without catalysts and with the presence of FFA. However, the FFA enhancement became less significant when the system was operated for a longer period of time than 120 min.

17/01708 Source-based discrete and continuous-time formulations for the crude oil pooling problem

Castro, P. M. *Computers & Chemical Engineering*, 2016, 93, 382–401.

The optimization of crude oil operations in refineries is a challenging scheduling problem due to the need to model tanks of varying composition with non-convex bilinear terms, and complicating logistic constraints. Following recent work for multiperiod pooling problems of refined petroleum products, a source-based mixed-integer non-linear programming formulation is proposed for discrete and continuous representations of time. Logistic constraints are modelled through generalized disjunctive programming while a specialized algorithm featuring relaxations from multiparametric disaggregation handles the bilinear terms. Results over a set of test problems from the literature show that the discrete-time approach finds better solutions when minimizing cost (avoids source of bilinear terms). In contrast, solution quality is slightly better for the continuous-time formulation when maximizing gross margin. The results also show that the specialized global optimization algorithm can lead to lower optimality gaps for fixed CPU, but overall, the performance of commercial solvers BARON and GloMIQO are better.

17/01709 Stabilisation/solidification and bioaugmentation treatment of petroleum drill cuttings

Kogbara, R. B. *et al. Applied Geochemistry*, 2016, 71, 1–8.

Petroleum drill cuttings are usually treated by techniques suitable for particular contaminant groups. The significance of this study consists in the development of a treatment technology that can simultaneously handle the hydrocarbon and metal constituents of drill cuttings. Bioaugmentation is combined with stabilization/solidification (S/S), within S/S monoliths and in granulated S/S monoliths. Portland cement was used for S/S treatment at 30% binder dosage. Bioaugmentation treatment involved two bacterial densities of a mixed culture biopreparation. The effects of inclusion of compost, fertilizer and activated carbon were also evaluated. After 28 days, the combined S/S and bioaugmentation treatments recorded up to 15% higher total petroleum hydrocarbon (TPH) loss than control S/S treatment without bioaugmentation. Embedding fertilizer, activated carbon and higher bacterial density within S/S monoliths resulted in the highest (99%) TPH reduction but higher concentrations of metals. The addition of compost and lower bacterial density to granulated S/S monoliths led to similar (98%) TPH degradation and lower amounts of metals. The results suggest that with better mixture optimization, combining S/S and bioaugmentation could engender more sustainable treatment of drill cuttings.

Economics, business, marketing, policy

17/01710 Country-specific oil supply shocks and the global economy: a counterfactual analysis

Mohaddes, K. and Pesaran, M. H. *Energy Economics*, 2016, 59, 382–399.

This paper investigates the global macroeconomic consequences of country-specific oil-supply shocks, providing a contribution that is both theoretical and empirical. On the theoretical side, the authors develop a model for the global oil market and integrate this within a compact quarterly model of the global economy to illustrate how this multi-country approach to modelling oil markets can be used to identify country-specific oil-supply shocks. On the empirical side, estimating the GVAR-Oil model for 27 countries/regions over the period 1979Q2 to 2013Q1, the authors show that the global economic implications of oil-supply shocks (due to, for instance, sanctions, wars, or natural disasters) vary considerably depending on which country is subject to the shock. In particular, it was found that adverse shocks to Iranian oil output are neutralized in terms of their effects on the global economy (real outputs and financial markets) mainly due to an increase in Saudi Arabian oil production. In contrast, a negative shock to oil supply in Saudi Arabia leads to an immediate and permanent increase in oil prices, given that the loss in Saudi Arabian production is not compensated for by the other oil producers. As a result, a Saudi Arabian oil supply shock has significant adverse effects for the global economy with real gross domestic product falling in both advanced and emerging economies, and large losses in real equity prices worldwide.

17/01711 Crude oil and stock markets: causal relationships in tails?

Ding, H. *et al. Energy Economics*, 2016, 59, 58–69.

This paper considers the causal relationships between WTI and Dubai crude oil returns and five stock index returns (S&P 500, Nikkei, Hang Seng, Shanghai, and KOSPI) within the quantile causality framework by using daily data for a period from 1 January 1996, to 12 October 2012. The quantile causality test is useful for a comprehensive understanding of the causal relationship between two returns. The test reveals several noteworthy results. First, although WTI returns are not closely related to Asian countries, some financial markets such as Nikkei and Hang Seng Granger-cause WTI returns. Second, the significance of causality from one market to another derives only from lower and upper levels of quantiles except for the case of causality from Nikkei to WTI returns. Third, all stock index returns Granger-cause Dubai crude oil returns over almost all quantile levels except for Shanghai returns. Fourth, Dubai crude oil returns Granger-cause all Asian stock index returns except for S&P 500 returns. Finally, the results indicate asymmetric causality from Dubai crude oil returns to Shanghai returns and KOSPI returns to Dubai crude oil returns.

17/01712 Downstream oil supply chain management: a critical review and future directions

Lima, C. *et al. Computers & Chemical Engineering*, 2016, 92, 78–92.

The oil industry has been playing a particular role in the modern economy, acting globally in different countries within competitive business environments. Due to the complexity of the oil supply chain, the associated decision making process is a difficult task, which involves numerous elements from oil supply, going through oil refining, up to oil product distribution. Thus, decision-support tools are often required to assist the decision making in the context of the oil supply chain. The improvement of such decision-support tools is a continuous goal for corporations. From this background, this work aims to review the scientific production about the application of mathematical programming techniques to the distribution problems, faced by diverse entities in the downstream oil supply chain. The main objectives are to point out main contributions, besides identifying the major voids and new trends in order to establish an agenda for future research directions.

17/01713 Dynamic structure of the spot price of crude oil: does time aggregation matter?

Aghababa, H. and Barnett, W. A. *Energy Economics*, 2016, 59, 227–237.

This paper assesses non-linear structures in the time series data generating mechanism of crude oil prices. The authors apply well-known univariate tests for non-linearity, with distinct power functions over alternatives, but with different null hypotheses reflecting the existence of different concepts of linearity and non-linearity in the time

series literature. They utilize daily data on crude oil spot price for over 26 years, as well as monthly data on crude oil spot price for 41 years. Investigating the monthly price of crude oil along with the daily price distinguishes the approach of this paper from existing studies focusing on the time series structure of crude oil price. All the tests detect strong evidence of general non-linear serial dependence, as well as non-linearity in the mean, variance, and skewness functions in the daily spot price of crude oil. Since evidence of non-linear dependence is less dramatic in monthly observations, non-linear serial dependence is moderated by time aggregation in crude oil prices but not significantly.

17/01714 Energy infrastructure modeling for the oil sands industry: current situation

Lazzaroni, E. F. *et al. Applied Energy*, 2016, 181, 435–445.

In this study, the total energy requirements associated with the production of bitumen from oil sands and its upgrading to synthetic crude oil (SCO) are modelled and quantified. The production scheme considered is based on the commercially applied steam-assisted gravity drainage (SAGD) for bitumen extraction and delayed coking for bitumen upgrading. In addition, the model quantifies the greenhouse gas (GHG) emissions associated with the production of energy required for these operations from technologies utilized in the currently existing oil sands energy infrastructure. The model is based on fundamental engineering principles, and Aspen HYSYS and Aspen Plus simulations. The energy demand results are expressed in terms of heat, power, hydrogen, and process fuel consumption rates for SAGD extraction and bitumen upgrading. Based on the model's output, a range of overall energy and emission intensity factors are estimated for a bitumen production rate of 112,500 BPD (or 93,272 BPD of SCO), which were determined to be 262.5–368.5 MJ/GJ_{SCO} and 14.17–19.84 gCO_2/MJ_{SCO}, respectively. The results of the model indicate that the majority of GHG emissions are generated during SAGD extraction (up to 60% of total emissions) due to the combustion of natural gas for steam production, and the steam-to-oil ratio is a major parameter affecting total GHG emissions. The developed model can be utilized as a tool to predict the energy demand requirements for integrated SAGD/upgrading projects under different operating conditions, and provides guidance on the feasibility of lowering GHG emissions associated with their operation.

17/01715 Impact of renewable and non-renewable energy consumption on economic growth: new evidence from the MENA net oil exporting countries (NOECs)

Kahia, M. *et al. Energy*, 2016, 116, 102–115.

This study explores the economic growth – energy consumption nexus for two samples of Middle East and North Africa (MENA) net oil exporting countries (NOECs) during the period 1980–2012. Using panel cointegration approach, strong evidence was found for the existence of a long-run relationship between real gross domestic product, renewable and non-renewable energy consumption, real gross fixed capital formation, and the labour force. Moreover, empirical results from the estimation of the panel error correction model indicate evidence of a unidirectional causality running from economic growth to renewable energy consumption in the short run. In the long run, the results show evidence of a bidirectional causality for the entire group of MENA NOECs. For the five selected MENA NOECs sample, strong evidence was found for bidirectional causality between renewable energy and economic growth. Additionally, these results confirm bidirectional causality between renewable and non-renewable energy consumption with negative and significant coefficient in the short-run indicating substitutability between these two types of energy. Finally, the paper discusses the economic implications of the results and proposes certain policies recommendations.

17/01716 Jojoba oil: a state of the art review and future prospects

Sánchez, M. *et al. Energy Conversion and Management*, 2016, 129, 293–304.

Jojoba oil, which is derived from the extraction of Jojoba seed, has a peculiar molecular structure in comparison with the rest of conventional oils. Jojoba oil is formed by long monounsaturated esters whereas the rest of the oils are usually composed by triglycerides. This unconventional structure confers to Jojoba oil unique properties and characteristics that are very valuable for fine chemical industry and for the production of pharmaceuticals. In addition, Jojoba oil can be an excellent source of fatty acid alkyl esters or biodiesel after the transesterification process and the purification steps. This review presents general information about the production of Jojoba oil and its derivatives, its composition, oil extraction process and the applications of this oil when it is used directly or after chemical transformation as well as the possible purposes of Jojoba meal after extraction. In addition, this paper contemplates the advantages and disadvantages of the use of homogeneous and heterogeneous catalysts for the Jojoba oil transesterification as well as different methods to obtain long monounsaturated alcohols, which have pharmaceutical applications, after being separated from biodiesel. The properties of the products derived from the transesterification of Jojoba oil are broadly discussed. Moreover, this review suggests future research opportunities such as a possible biorefinery using Jojoba oil as main raw material, supercritical methods and simultaneous extraction/reaction process which are fully discussed.

17/01717 Mass and energy-capital conservation equations to forecast the oil price evolution with accumulation or depletion of the resources

Gori, F. *Energy*, 2016, 116, 746–760.

The present work extends the approach of using the mass and energy-capital conservation equations to forecast the price evolution of oil when accumulation or depletion is present. The price evolution is then dependent on the consumption rate of the oil, besides the ratio of mass extraction to mass consumption rates, and the usual economic parameters, e.g. the interest rates of non-extracted and extracted resources. The main conclusions are that a ratio of mass extraction to consumption rates different from unity, i.e. when accumulation or depletion of the oil is present, can modify the approach of the oil price forecast without accumulation or depletion of the resources.

17/01718 Oil prices and global factor macroeconomic variables

Ratti, R. A. and Vespignani, J. L. *Energy Economics*, 2016, 59, 198–212.

This paper investigates the relationship between oil prices, global industrial production, prices, central bank policy interest rate and monetary aggregate with a global factor-augmented error correction model. The authors confirm the following stylized relationships: (i) at global level, money, industrial production and prices are cointegrated; (ii) positive innovation in global oil price is connected with global interest rate tightening; (iii) positive innovation in global money, price level and industrial production is connected with an increase in oil prices; (iv) positive innovations in global interest rate are associated with a decline in oil prices; and (v) the USA, the Euro area and China are the main drivers of global macroeconomic factors.

17/01719 Optimized integration of renewable energy technologies into Alberta's oil sands industry

Elsholkami, M. *et al. Computers & Chemical Engineering*, 2016, 90, 1–22.

An energy optimization model for the integration of renewable technologies into the energy infrastructure of the oil sands industry is presented. The proposed model determines the optimal configuration of oil producers and the energy infrastructure required to meet their energy demands. The model is geared toward the minimization of cost subject to carbon dioxide emission constraints. A mixed integer non-linear optimization model is developed that simultaneously optimizes capacity expansion and new investment decisions of conventional and renewable energy technologies. To illustrate its applicability, the proposed model was applied to a case study using data reported in the literature for various years of oil sands operations. A rolling horizon approach was implemented to determine the effect of investment decisions of previous operational years on the selection of new investment options. Results were compared with and without the incorporation of renewable energy technologies. The results obtained indicate that the proposed model is a practical tool that can be employed to evaluate and plan oil sands and energy producers for future scenarios. Moreover, the results show that renewable energy technologies have significant potential in reducing reliance on fossil-fuel based technologies and their associated CO_2 emissions. The emission constraints set for the operational year 2025 can only be achieved by the incorporation of renewables in the energy production mix.

17/01720 Small-scale production of hydrous ethanol fuel: economic and environmental assessment

Mayer, F. D. *et al. Biomass and Bioenergy*, 2016, 93, 168–179.

Energy consumption in rural areas and the increasing demand for liquid fuels in Brazil has stimulated the development of alternatives for fuels production, including ethanol. The potential of small-scale ethanol production (SSEP) – up to 5000 L daily – can help to meet this demand and contribute byproducts to animal feed. This study aims to assess the economic feasibility and environmental impacts of ethanol production at a small-scale distillery with a production capacity of 30 $L\,h^{-1}$ of hydrous ethanol fuel (HEF). Regarding cost, three cases were analysed in which the minimum, average and maximum raw material prices were assessed. The cost of HEF for these cases was US$0.68, 0.92 and 1.16 per litre, respectively, highlighting the cost of the raw materials, which can contribute up to 69% of the total cost. Life cycle Assessment shows that agricultural stage is responsible for higher environmental impact in 7 of 11 categories, requiring special attention to minimize potential damage. SSEP has positive energy balance (1.97)

only considering bagasse silage as byproduct or replacing firewood by bagasse to generate process heat (7.39). This study demonstrates that without the support of policies that provide economic incentives for HEF production, the small-scale production of HEF will have a secondary role in supplying HEF to meet the demand for liquid fuels in Brazil.

17/01721 Statistical properties of country risk ratings under oil price volatility: evidence from selected oil-exporting countries

Liu, C. *et al. Energy Policy*, 2016, 92, 234–245.

This paper focuses on the application of panel models for identification and analysis of influence of oil price volatility on statistical properties of country risk ratings which stem from uncertainty of macroeconomic fluctuations. Firstly, two statistical properties of country risk ratings, volatility clustering and asymmetrical revision were identified in a theoretical framework. Secondly, considering the oil price volatility, numerical experiments were conducted based on extended models to test and verify specific properties of country risk ratings in selected oil-exporting countries. Empirical results suggest that properties of country risk remain comparatively steady despite oil price volatility. It is also found that the oil price volatility can obviously exaggerate the country risk volatility, as it happened during 2007–2009. Country clustering based on the properties of country risk ratings shows that the selected countries maintain a significant clustering tendency. These features are of great importance for estimating risk exposure of international trade and investments in oil export during extreme situations.

17/01722 The informational content of inventory announcements: intraday evidence from crude oil futures market

Ye, S. and Karali, B. *Energy Economics*, 2016, 59, 349–364.

This paper examines the behaviour of intraday crude oil futures return and volatility and how they respond to weekly inventory announcements by the American Petroleum Institute (API) and Energy Information Administration (EIA). The informational content of API reports is measured relative to market analysts' expectations collected by Reuters, whereas that of EIA reports is measured relative to API reports. Results suggest that unexpected inventory changes in both API and EIA reports exert an immediate inverse impact on returns and a positive impact on volatility; but the duration and magnitude of EIA inventory shocks are longer and larger, with the largest impact observed when Reuters and API both err on the same side. While there are no instant asymmetric return responses to positive and negative API shocks, the return and volatility responses to cross-commodity inventory shocks in EIA reports exhibit asymmetry.

Derived liquid fuels

17/01723 Capturing rents from natural resource abundance: private royalties from U.S. onshore oil & gas production

Brown, J. P. *et al. Resource and Energy Economics*, 2016, 46, 23–38.

This study considers how much private mineral owners capture geologically driven advantages in well productivity through a higher royalty rate. Using proprietary data from nearly 1.8 million leases, the authors estimate that the six major shale plays generated $39 billion in private royalties in 2014. There is limited pass-through of resource abundance into royalty rates. A doubling of the ultimate recovery of the average well in a county increases the average royalty rate by 1–2 percentage points (a 6–11% increase). Thus, mineral owners benefit from resource abundance primarily through a quantity effect, not through negotiating better lease terms from extraction firms. The low pass-through likely reflects a combination of firms exercising market power in private leasing markets and uncertainty over the value of resource endowments.

17/01724 Clean co-production of H_2 and power from low rank coal

Aziz, M. *et al. Energy*, 2016, 116, 489–497.

This work proposes a state-of-the art integrated system for the co-production of H_2 and power from low rank coal with high total energy efficiency. A model of this system is developed based on enhanced process integration technology, incorporating coal drying, gasification, chemical looping, power generation, and hydrogenation. In this model, heat circulation and process integration technologies are effectively combined, minimizing the exergy losses. Iron-based materials are used as oxygen carriers and are circulated in a chemical looping module consisting of three continuous processes: reduction, oxidation, and combustion. The toluene–methyl cyclohexane system is employed as a liquid organic H_2 carrier to store H_2 generated from coal. The effects of the fluidization velocity in drying, the steam-to-fuel ratio in gasification, and the chemical looping pressure are evaluated with regard to the power generation and H_2 production efficiencies as well as the overall efficiency, and the proposed integrated system exhibits very high efficiencies of approximately 12%, 72% and 84%, respectively.

17/01725 Enhanced butanol production by solvent tolerance *Clostridium acetobutylicum* SE25 from cassava flour in a fibrous bed bioreactor

Li, H.-g. *et al. Bioresource Technology*, 2016, 221, 412–418.

To enhance the butanol productivity and reduce the material cost, acetone, butanol and ethanol fermentation by *Clostridium acetobutylicum* SE25 was investigated using batch, repeated-batch and continuous cultures in a fibrous bed bioreactor, where cassava flour was used as the substrate. With periodical nutrient supplementation, stable butanol production was maintained for about 360 h in a six-cycle repeated-batch fermentation with an average butanol productivity of 0.28 g/L/h and butanol yield of 0.32 g/g-starch. In addition, the highest butanol productivity of 0.63 g/L/h and butanol yield of 0.36 g/g-starch were achieved when the dilution rate were investigated in continuous production of acetone, butanol, and ethanol using a fibrous bed bioreactor, which were 231.6% and 28.6% higher than those of the free-cell fermentation. On the other hand, this study also successfully confirmed that the biofilm can provide an effective protection for the microbial cells which are growing in stressful environment.

17/01726 Mass transfer simulation of biodiesel synthesis in microreactors

Pontes, P. C. *et al. Computers & Chemical Engineering*, 2016, 93, 36–51.

A coupled non-linear mathematical model for the mass transfer of the species involved in the transesterification reaction between soybean oil and methanol in a parallel plates geometry microreactor is presented. The set of partial differential equations that governs the concentration profile of these species were obtained from the general mass balance equation for the case of isothermal flow and steady state with constant physical properties. The velocity profile was obtained from the Navier–Stokes equations assuming fully developed stratified laminar flow for two immiscible Newtonian fluids, with a plane interface between them, based on experimental observation of this flow pattern. The second-order kinetic equations for the species were developed assuming homogeneous and reversible chemical reactions and these equations were written as source terms in the main equations. The mathematical model was solved using the hybrid method known as generalized integral transform technique. The simulation results were critically compared with those obtained by using the COMSOL multiphysics platform, showing a good agreement between the hybrid and fully numerical simulations. The effects of governing parameters such as residence time, temperature and microreactor dimensions were investigated. It was observed that higher triglycerides conversion rates occurred at higher temperatures and residence times and lower microreactor depths.

17/01727 Methodology for solar and wind energy chemical storage facilities design under uncertainty: methanol production from CO_2 and hydrogen

Martín, M. *Computers & Chemical Engineering*, 2016, 92, 43–54.

Production facilities that store solar or wind energy in the form of chemicals present underused capacity. The problem needs to address uncertain and variable operating conditions and prices for complex process models. A mixed-integer linear programming formulation is developed including surrogate models based on the detailed non-linear programming steady-state models. The model solves the trade-offs between investment and production capacity. This approach is applied to the case of the production of methanol from CO_2 and solar or wind based hydrogen. Two cases are evaluated, Spain and UK. For the Spanish case, if electricity can be sold and there is no area restrictions, the process produces an excess of electricity with the solar panels available during summer time. Otherwise, electricity is only produced when excess capacity is available. In the UK, only wind turbines are used and the excess of electricity is produced during winter time.

17/01728 Optimization of packing state in brown coal water slurry based on the two-grade fractal model

Yang, X. *et al. Fuel*, 2016, 168, 54–60.

A newly designed two-grade fractal model for improving the packing state in brown coal water slurry (BCWS), which was built on the fractal theory and modified by separating the size into two grades, was investigated systematically. Packing efficiency (PE) and regression levels of the fractal model in various particle systems were analysed. The results showed that the PE of brown coal particle system is determined mainly by the fractal characteristics of particles under 74 μm and the packing state in BCWS can be significantly improved when the fractal dimension is around 2.6–2.7. In addition, the two-grade fractal model fits the PSDs for various particle systems with

different graduation ratios of coarse samples (CS), fine samples (FS) and ultra-fine samples (UFS) well. PE reaches the maximum value when the graduation ratio is 7 : 0 : 3 (CS : FS : UFS) and the fractal dimension is 2.7080, which is consistent with the calculated results. It was confirmed by the slurry preparation experiment that the maximum solid loading of BCWS increased by 2.9% through optimizing the packing state using two-grade fractal model.

17/01729 Production of aromatic hydrocarbons via catalytic co-pyrolysis of torrefied cellulose and polypropylene
Lee, H. W. *et al. Energy Conversion and Management*, 2016, 129, 81–88.
The effects of the torrefaction of cellulose on catalytic co-pyrolysis with polypropylene (PP) over HZSM-5 and HBeta catalysts were examined in a pyrolyser-GC/MS/TCD/FID system. Torrefied cellulose produced larger quantities of aromatic hydrocarbons during catalytic pyrolysis over both BETA and HZSM-5 catalysts than raw cellulose due to the change in crystallinity and structure of cellulose. Among the catalysts tested, HZSM-5(30) showed the highest performance for the production of aromatic hydrocarbons from the catalytic pyrolysis of torrefied cellulose. The synergy effect for the production of aromatic hydrocarbons was also observed on the catalytic co-pyrolysis of torrefied cellulose and PP over HZSM-5, even when a low catalyst to sample ratio was applied. The maximum BTEXs yield (33.4 wt%) was achieved from the catalytic co-pyrolysis of torrefied cellulose and PP at a catalyst to sample ratio of 3/1 and a torrefied cellulose to PP ratio of 1/3.

17/01730 Robust surface-modified Beta zeolite for selective production of lighter fuels by steam-assisted catalytic cracking from heavy oil
Khalil, U. *et al. Fuel*, 2016, 168, 61–67.
Production of lighter hydrocarbons were maximized by steam-assisted catalytic cracking of heavy oil over silane treated Beta catalysts. Steaming environment may cause dealumination of zeolites and affect the stability of zeolites. Herein, the authors improved the hydrophobicity and stability of the Beta zeolite catalyst ($SiO_2/Al_2O_3 = 150$) by modifying its surface using triphenyl silane through vapour phase deposition technique. Parent Beta and silane treated Beta catalysts were tested in fixed-bed flow reactor for steam-assisted catalytic cracking of atmospheric residue. It was found that the modified Beta catalyst retained its crystallinity and phase purity after reaction. Moreover, coke formation was also reduced significantly over silane treated Beta catalysts. This indicates the increase in the stability of catalysts. Furthermore, the yields of gases, gasoline (C_7–C_{13}) and gas oil (C_{14}–C_{20}) over a silane treated Beta zeolite catalyst were 11.6, 55.7 and 3.7 mol% respectively for 2 h reaction time.

17/01731 Surface tension and rheological behavior of sal oil methyl ester biodiesel and its blend with petrodiesel fuel
Hajra, B. *et al. Fuel*, 2016, 166, 130–142.
This paper deals with experimental and theoretical investigation of surface tension, apparent viscosity and viscoelastic properties of sal oil methyl ester biodiesel and its blends with petrodiesel at different temperature. Several methods were used to predict surface tension and apparent viscosity of biodiesel–petrodiesel blends. Satri–Rao method based on the corresponding state predicts surface tension of biodiesel–petrodiesel blends very well, whereas UNIFAC–VISCO group contribution method predicts apparent viscosity of blends very accurately. To predict the apparent viscosity of biodiesel, six unknown UNIFAC–VISCO group interaction parameters were determined and proposed parameters were then used to predict viscosities of biodiesel–petrodiesel blends. The recommendation was given which as to the proportion of sal oil biodiesel and normal diesel to be mixed to get the proper European standard grade diesel fuel. Viscoelastic properties (i.e. structural stability, storage modulus, loss modulus, complex viscosity and loss tangent) of biodiesel–petrodiesel blends were determined as a function of amplitude, frequency and temperature using parallel plates rotational viscometer in linear viscoelastic range. Finally, generalized Cox–Merz parameters were used to establish the relation between apparent viscosity and complex viscosity of blends.

17/01732 Wood residue (*Pinus patula* bark) as an alternative feedstock for producing ethanol and furfural in Colombia: experimental, techno-economic and environmental assessments
Moncada, J. *et al. Chemical Engineering Science*, 2016, 140, 309–318.
This study investigates the technical, economic and environmental performances for producing ethanol and furfural from *Pinus patula* bark, on a biorefinery concept. This was done through experimental, techno-economic and environmental assessments. The experimental analysis considered the physicochemical characterization of the raw material and three pre-treatment methods: (i) dilute acid, (ii) alkali and (iii) liquid hot water. The alkali method showed the highest yield (50%) and the pentose rich hydrolysate was used to produce furfural (yield 91%). The solid from the pre-treatment stage was enzymatically hydrolysed (maximum concentration 63 g/l), and the hexose-rich solution was used as substrate for producing ethanol (0.42 g ethanol/g sugars). The obtained experimental yields were used as the basis to build a process model to generate mass and energy balances, from which the techno-economic and environmental assessments are derived. Based on different levels of heat integration, three scenarios were assessed: (scenario 1) non-integrated, (scenario 2) fully energy integrated and (scenario 3) fully integrated plus cogeneration scheme. Results revealed that by increasing the level of energy integration, the biorefinery system can be profitable with a positive net present value (scenario 3: US$184.54 million/y) and a payout period within the project's life-time (scenario 3: 2.22 years). The annualized production costs can be decreased up to 84% and 66% for scenario 3 in comparison to scenarios 1 and 2, respectively. From the environmental point of view, the biorefinery system is positively affected by increasing the level of energy integration. The potential environmental impact can be reduced up to 74% and 66% for scenario 3, in comparison with scenarios 1 and 2, respectively.

03 GASEOUS FUELS

Sources, properties, recovery, treatment

17/01733 Assessing groundwater-surface water connectivity using radon and major ions prior to coal seam gas development (Richmond River Catchment, Australia)
Atkins, M. L. *et al. Applied Geochemistry*, 2016, 73, 35–48.
Coal seam gas (CSG, or coal bed methane) mining is rapidly growing, with poorly understood impacts on groundwater and surface water systems. Here, chemical tracers were used to investigate groundwater-surface water connectivity in an Australian river system (Richmond River Catchment, New South Wales) prior to CSG extraction but after ~50 exploratory CSG wells were drilled. The authors performed four surveys of 29 interconnected creek and river sites, over contrasting hydrological conditions. Radon was used to determine if a surface water segment was gaining groundwater. Radon observations over four seasons revealed that 28 out of 77 surface water segments were clearly gaining groundwater, five were possibly gaining groundwater and 44 were undetermined. This is equivalent to gaining segments in 333 km (39%) of surface water from the 864 km being investigated. High spatial and temporal variability in groundwater gaining segments was found. Na/Cl ratios were used to determine the fraction of groundwater in surface water. Overall, the groundwater contribution in surface waters was 14–24% higher in post-flood conditions than during the other three surveys of baseflow and moderate flow conditions. The results serve as a regional baseline assessment of river water chemistry and groundwater-surface water connectivity prior to the planned development of CSG fields. The geochemical tracer approach allows for a quick qualitative assessment of groundwater-surface water connectivity in poorly gauged river systems and can define priority locations where groundwater extraction for CSG mining should be carefully managed.

17/01734 Experimental investigation of condensation heat transfer and pressure drop of propane, R1234ze(E) and R22 in minichannels
Liu, N. *et al. Applied Thermal Engineering*, 2016, 102, 63–72.
The paper reports measured heat transfer and pressure drop data for condensation of propane, R1234ze(E) and R22 in circular ($d_h = 1.085$ mm) and square ($d_h = 0.952$ mm) horizontal minichannels. The saturation temperatures are 40 and 50 °C with mass fluxes varying from 200 to 800 kg/(m^2 s) and vapour qualities from 0.1 to 0.9. The experiments investigated the effects of mass flux, vapour quality, saturation temperature and channel geometry on the heat transfer coefficients and pressure drops. The results show that the heat transfer coefficients and pressure drops increase with increasing mass flux and vapour quality and decreasing saturation temperature. The heat transfer coefficients in the square minichannel are larger than those in the circular minichannel. The study shows that propane and R1234ze(E) are good substitutes for R22 based on the condensation heat transfer characteristics. The pressure gradients in the circular and square minichannels differ little for propane with mass fluxes of 200, 350 and 500 kg/(m^2 s) and for R1234ze(E) with a mass flux of 500 kg/(m^2 s). The pressure gradients for propane are larger than those of

R1234ze(E) which are larger than those of R22. Condensation heat transfer and two-phase pressure drop correlations were evaluated against the experimental data in the square minichannel.

17/01735 Free hydrogen-hydrocarbon gases from the Lovozero loparite deposit (Kola Peninsula, NW Russia)

Nivin, V. A. *Applied Geochemistry*, 2016, 74, 44–55.

The Lovozero nepheline-syenite massif in the north-eastern Fennoscandian Shield, well-known to mineralogists and petrologists, is also interesting with its high contents of hydrogen-hydrocarbon gases in different forms of presence, which is untypical of magmatic rocks. The paper systematizes and generalizes little known and unpublished data on the composition, location, character and scale (intensity) of the free gases (FG) emission within a major loparite deposit confined to the massif. CH_4 and H_2 are dominant in the FG composition. The molecular weight distribution of hydrocarbon gas components corresponds to the classic Anderson–Schulz–Flory distribution with a steep gradient. Carbon and hydrogen of the gases are characterized by rather heavy isotope compositions, becoming lighter from the transition of methane to ethane. The FG volume has been estimated as 0.2–1.6 m^3 of gas per 1 m^3 of undisturbed rock. The gas recovery of walls in underground workings has been up to 0.2 ml/min/m^2 for CH_4 and 0.5 ml/min/m^2 for H_2 in several years after their heading. The discharge of some shot holes that characterizes the gas emission intensity (1.8–2 m deep and 40 mm in diameter) is up to 300 ml/min, but it is one or two orders lesser values dominate. The discharge time in some sections varies from several days to 20 years. The overpressure of gases towards the air mainly does not increase 100 hPa, sometimes reaching 120 kPa. It has been defined, that FG distribute irregularly (at the distance of centimetres to hundreds of metres) and their composition and particularly emission intensity perform different temporal fluctuations. The abiogenic origin of FG has been proposed, with FG appearing as a mixture of gases in various proportions: (a) gases remaining in microfissures at the massif's consolidation after the capture by fluid inclusions and those lost during degassing and (b) gases occurred in mechanic-chemical reactions, partial emission and concentration of occluded and diffusely scattered gases under the unstable stress-strain mode of the rock mass. Combustible and explosive hydrogen–hydrocarbon FG can accumulate in the air of underground workings and cause accidents, disrupting the workflow. The background for using characteristics of spatial-temporal variations of the FG emission as precursors of dangerous geodynamic phenomena has been indicated.

17/01736 Simple petrographic grain size analysis of siltstone reservoir rocks: an example from the Montney tight gas reservoir (western Canada)

Sanei, H. *et al. Fuel*, 2016, 166, 253–257.

This paper presents a simple petrographic approach to measure grain size distributions of fine-grained tight reservoir rocks, simultaneous to other organic petrographic measurements. Application of reflected light microscopy on polished blocks is a routine methodology for organic petrographic analyses including maceral examination and measurement of vitrinite reflectance. While routine petrographic analysis is in progress, the presented method enables operators to provide simultaneous reporting of quantitative grain size distribution by random orientation measurement of grain diameters using a relatively quick and simple procedure. This method provides added value to the routine analytical information provided by organic petrography laboratories. Application of ultra violet (UV) incident light under both oil and water immersion objectives provides a far better visual distinction of grain boundaries compared to white incident light. The improved visual distinction is likely due to differences in the diffused UV energy between surface scattering of the crystalline grains and the subsurface scattering of the incident light from internal irregularities such as grain boundaries and cemented areas in the polycrystalline rock samples. As a result of this optical phenomenon, grain boundaries are highly visible as a light blue UV rim. The authors suggest a random orientation measurement of 50–250 grain diameters, depending on sample sorting in various parts of a polished block, to give a valid statistical dataset and a valid size distribution histogram.

17/01737 Structural properties of methane and butane mixed-gas hydrates

Kida, M. *et al. Chemical Engineering Science*, 2016, 140, 10–15.

Solid-state ^{13}C NMR and powder X-ray diffraction measurements were conducted on mixed gas hydrates including methane and butane (*i*-butane and *n*-butane) to investigate the effect of guest composition in the hydrate lattice on the lattice parameters and density. The guest molecules were quantitatively analysed by ^{13}C NMR spectroscopic techniques without the influence of uncaged components. The ^{13}C NMR measurements showed that the large cages in the structure II hydrate framework were almost fully occupied by methane and butane. Furthermore, small cage occupancies decreased with increasing butane composition as butane molecules preferentially occupied the large cages of structure II. The powder X-ray diffraction profiles showed that the lattice constant of structure II hydrate crystals increased with increasing butane composition, suggesting that the variation in guest distribution in the methane–butane systems contributes to the lattice expansion. The hydrate densities were estimated using the lattice parameters from the powder X-ray diffraction profiles and cage occupancies from ^{13}C NMR spectra, and the results obtained suggested that the lattice expansion contributes to lowering the hydrate density. The resultant structural properties of the mixed gas hydrates will be useful for designing novel gas hydrate technologies.

17/01738 The cost of unconventional gas extraction: a hedonic analysis

Delgado, M. S. *et al. Resource and Energy Economics*, 2016, 46, 1–22.

This study focuses on the identification and estimation of potentially negative environmental impacts of unconventional natural gas extraction on property values in the USA and advance previous research by contributing new data and new identification strategies for isolating these potential impacts. The study area consists of two counties in Pennsylvania that are home to large amounts of unconventional natural gas extraction but are otherwise isolated from other resource extraction industries or large urban areas. Parametric, semi-parametric, and matching hedonic regression models were deployed that included recent quasi-experimental methods and, in contrast to previous research and much popular intuition, the authors failed to find robust significance that negative environmental externalities of natural gas extraction were reflected in nearby property values. While there may be plausible risks associated with unconventional natural gas extraction, the authors did not find consistent evidence to suggest that these risks significantly affect nearby property values.

Transport, storage

17/01739 A semi-analytical method of stress-strain analysis of buried steel pipelines under submarine landslides

Zhang, L. *et al. Applied Ocean Research*, 2016, 59, 38–52.

A semi-analytical method of the stress-strain analysis of buried steel pipelines under submarine landslides was proposed, considering the non-linearities of the pipe–soil interaction and mechanical properties of the pipe steel. The pipeline was divided into three parts according to different loading conditions, and the corresponding differential equations were established based on a combination of the beam-on-elastic foundation and elastoplastic-beam theories. According to the second-order central difference method, the transverse horizontal displacement was calculated, and then the bending strain was obtained based on the relation between bending strains and curvatures. Considering the interaction between the axial and bending strains, the axial strain can be derived from the equilibrium condition by equating the axial force. The proposed method was verified through the comparison of obtained solutions to ANSYS results, with minor deviations which do not exceed about 4.6%. Additionally, the effects of the slide width, the buried depth of pipelines, the internal friction angle of soils, the cohesion of soils and the bulk density of soils are investigated through parametric studies.

17/01740 Multi-objective design optimization of natural gas transmission networks

da Silva Alves, F. *et al. Computers & Chemical Engineering*, 2016, 93, 212–220.

This paper proposes the multi-objective optimization of the design of natural gas transmission networks to support the decision of regulatory authorities. The problem formulation involves two objective functions: the minimization of the transportation fare and the maximization of the transported gas volume. These design parameters of the pipeline project must be previously established by the regulatory agency, considering an attractive return on the investment for the entrepreneurs and the demands of current and future consumers. The solution of this problem without an optimization tool may imply in unfair gas prices or the lack of investor interest. The proposed analysis is focused on growing markets, associated to a continuous increase of the natural gas consumption. Constraints associated to gas flow and compressor stations guarantee the feasibility of the set of design options found. Aiming to illustrate the performance of the proposed approach, the tool was applied to a typical trunkline example.

17/01741 Simulation of methane adsorption and diffusion in a carbon nanotube channel

Yeganegi, S. and Gholampour, F. *Chemical Engineering Science*, 2016, 140, 62–70.

The effect of pore-connectivity feature of nanoporous carbons (NPCs) on the adsorptive and diffusive behaviour of methane was studied by a simple constricted carbon nanotube (C-CNT) model using grand canonical Monte Carlo and molecular dynamics simulations. In spite of slight overprediction, C-CNT model can properly predict the adsorption of methane in some real NPCs. The calculated heat of adsorption was well agreed with the reported values for the hypothetical Schwarzite (C_{168}) model and activated carbon. The obtained results show that the most preferred site for the adsorption of methane is the constricted region of the pore. The effect of constriction length on the methane uptake was studied at various pressures. It was shown that at low pressures the methane uptake increased with the length of constriction, while at high pressures the uptake is larger for short constriction. The diffusion coefficients of methane inside the C-CNT were calculated by very long MD simulations (220 ns). The calculated methane diffusion coefficients in the C-CNT were one to two orders of magnitude lower than that in the regular slit pores as well as the straight carbon nanotubes. In addition, the diffusion coefficients in the C-CNT were in the same order of magnitude as in the constricted slit and virtual porous carbon (VPC) models of carbon pores. MD simulations revealed that the diffusivity decreases with the constriction length and approaches a constant value for large constriction length.

Economics, business, marketing, policy

17/01742 An optimization framework for the integration of water management and shale gas supply chain design

Guerra, O. J. *et al. Computers & Chemical Engineering*, 2016, 92, 230–255.

This study presents the mathematical formulation and implementation of a comprehensive optimization framework for the assessment of shale gas resources. The framework simultaneously integrates water management and the design and planning of the shale gas supply chain, from the shale formation to final product demand centres and from fresh water supply for hydraulic fracturing to water injection and/or disposal. The framework also addresses some issues regarding wastewater quality, i.e. total dissolved solids (TDS) concentration, as well as spatial and temporal variations in gas composition, features that typically arise in exploiting shale formations. In addition, the proposed framework also considers the integration of different modelling, simulation and optimization tools that are commonly used in the energy sector to evaluate the technical and economic viability of new energy sources. Finally, the capabilities of the proposed framework are illustrated through two case studies (A and B) involving five well-pads operating with constant and variable gas composition, respectively. The effects of the modelling of variable TDS concentration in the produced wastewater is also addressed in case study B.

17/01743 Domestic LPG interventions in South Africa: challenges and lessons

Kimemia, D. and Annegarn, H. *Energy Policy*, 2016, 93, 150–156.

A majority of grid-connected households in South Africa use electricity for cooking and heating tasks. This thermal intensive use of electricity has a high load factor and is a contributory factor of electricity demand outstripping supply at peak demand periods. The government has promoted liquefied petroleum gas (LPG) as an alternative thermal energy source for household cooking and heating. This study evaluates the long-term successes, challenges and social impacts of an LPG intervention project that was piloted in Atteridgeville Township, a typical low-income suburb. The data was gathered through one-on-one household interviews with a sample of the beneficiaries. The results indicate that seven years after the LPG intervention, about 70% of the beneficiaries continue to use LPG and report that the intervention has improved their welfare. Fast cooking is cited as the key tangible benefit of LPG technology in households, followed by saving on electricity bills. The project would have achieved more success through better community engagement, including strict beneficiary selection criteria; a long-term LPG distribution and maintenance plan; and inclusion of recurring monthly LPG subsidies for indigent households. The study discusses the subset of factors necessary for successful rollouts of similar energy projects.

17/01744 How did the US economy react to shale gas production revolution? An advanced time series approach

Bilgili, F. *et al. Energy*, 2016, 116, 963–977.

This paper aims at examining the impacts of shale gas revolution on industrial production in the USA. To this end, this paper, first, throughout literature review, exposes the features of shale gas revolution in the USA in terms of energy technology and energy markets. However, the potential influences of shale gas extraction on the US economy are not explicit in the existing literature. Thus, considering mainly the output of shale gas revolution on the US economy in this research, later, the paper conducts econometric models to reveal if there exists significant effect(s) of shale gas revolution on the US economy. Therefore, the paper employs unit root tests and cointegration tests by following relevant US monthly data from January 2008 to December 2013. Then, this paper observes long-run impact of shale gas production on industrial production in the USA through dynamic ordinary least squares estimation with dummy structural breaks and conducts Granger causality test based on vector error correction model. The dynamic ordinary least squares estimator explores that shale gas production has a positive effect on industrial production. Besides, the Granger causality test presents that shale gas production Granger causes industrial production in the long run. Based on the findings of the long-run estimations, the paper yields that industrial production is positively related to shale gas production. Eventually, on its findings, this paper asserts that (i) the shale gas revolution in the US has considerable positive effects on the US economy within the scope of the validity of the growth hypothesis, (ii) new technologies might be developed to mitigate the possible negative environmental effects of shale gas production, (iii) the countries having shale gas reserves, as in USA, may follow energy policies to utilize their shale reserves more in the future to meet their energy demand and to increase their economic welfare.

17/01745 Impact of rent-seeking on productivity in Chinese coal mine safety supervision: a simulation study

Chen, H. *et al. Energy Policy*, 2016, 93, 315–329.

During the 'golden decade' (2001–2011) of the coal industry in China, rent-seeking increased in coal mine safety supervision alongside significant improvements in coal mine safety status and increased economic benefits in the coal industry. To explore this internal relationship, A Matlab simulation system was developed that simulated the impact of rent-seeking from each level of the supervision department on coal mine productivity in different scenarios. The results showed the following. (1) Rent-seeking had no significant influence on the average level of material productivity but it had an adverse effect on the average level of mental productivity. Due to the effects of rent-seeking, productivity tended to exhibit unstable and destructive fluctuations, and rent-seeking had the dual effect of promoting and restraining productivity in a wide range with a high frequency. (2) In the supervision scenario, supervision by the high-level department was efficient, and productivity was promoted more by the national and provincial supervision department. (3) In the rent-seeking scenario, each level of the department had an intensity threshold above which coal mine accidents occurred. Suggestions were also proposed that focused on the improved supervision of Chinese coal mine safety in three areas based on the 'new normal' safety concept.

17/01746 Model for forecasting residential heat demand based on natural gas consumption and energy performance indicators

Spoladore, A. *et al. Applied Energy*, 2016, 182, 488–499.

The forecasting of energy and natural gas consumption is a topic that spans different temporal and spatial scales and addresses scenarios that vary significantly in consistency and extension. Therefore, although forecasting models share common aims, the specific scale at which each model has been developed strongly impacts its features and the parameters that are to be considered or neglected. There are models designed to handle time scales, such as decades, years, and months, down to daily or hourly models of consumption. Similarly, there are patterns of forecasted consumption that range from continents or groups of nations down to the most limited targets of single individual users, passing through all intermediate levels. This paper describes a model that is able to provide a short-term profile of the hourly heat demand of end-users of a district heating network (DHN). The simulator uses the hourly natural gas consumptions of large groups of users and their correlation with the outside air temperature. Next, a procedure based on standards for estimating the energy performance of buildings is defined to scale results down to single-user consumption. The main objective of this work is to provide a simple and fast tool that can be used as a component of wider models of DHNs to improve the control strategies and the management of load variations. The novelty of this work lies in the development of a plain algebraic model for predicting hourly heat demand based only on average daily temperature and historical data of natural gas consumption. Whereas aggregated data of natural gas consumption for groups of end users are measured hourly or even more frequently, the thermal demand is typically evaluated over a significantly longer time horizon, such as a month or more. Therefore, the hourly profile of a single user's thermal demand is commonly unknown, and only long-term averaged values are available and predictable. With this model, used in conjunction with common weather forecasting services that reliably provide the average temperature of the following day, it is possible to predict the expected hourly heat demand one day in advance and day-by-day.

17/01747 The price and income elasticities of natural gas demand: international evidence

Burke, P. J. and Yang, H. *Energy Economics*, 2016, 59, 466–474.

Natural gas contributes a growing share of the world's energy mix. This study uses national-level data for a sample of 44 countries to estimate the price and income elasticities of natural gas demand. This paper presents both single-equation results and results instrumenting natural gas prices with proved natural gas reserves. This instrument includes both domestic reserves and distance-weighted reserves in other countries. Estimates were obtained of the average long-run price elasticity of natural gas demand of around −1.25 and of the average long-run income elasticity of natural gas demand of +1 and higher. Separate estimates were also presented for final natural gas demand by industry and households.

17/01748 The regional impact of a CO_2 tax on gasoline demand: a spatial econometric approach

Filippini, M. and Heimsch, F. *Resource and Energy Economics*, 2016, 46, 85–100.

In order to reduce CO_2 emissions and mitigate climate change, several countries around the world have introduced a CO_2 tax on energy consumption. Switzerland has already introduced a CO_2 tax on gas and heating oil and is considering introducing a CO_2 tax on gasoline and diesel as well. The effectiveness of such a tax depends on the level of the short- and long-run price elasticity. Moreover, acceptance of a CO_2 tax by a society depends on both the distributional effects of such a tax among households and its spatial effects among regions. In this paper, the regional impact of a hypothetical CO_2 tax on gasoline consumption in Switzerland is analysed by estimating a demand function for gasoline using panel data from 547 Swiss municipalities from 2001 to 2008. Gasoline sales were collected from the five largest gasoline companies operating in Switzerland, covering about 60% of overall sales. Swiss municipalities are relatively small units, and car ownership and use in one municipality is thought to influence gasoline sales in the neighbouring ones. Accordingly, the method used in the model also accounts for spatial correlation in the consumption of gasoline. Overall, this spatial econometric analysis shows that the tax burden of a CO_2 tax will be higher in rural areas than in urban areas.

Derived gaseous fuels

17/01749 Computational optimization and sensitivity analysis of fuel reformer

Raoufi, A. *et al. Computers & Chemical Engineering*, 2016, 93, 266–283.

In this study, the catalytic partial oxidation of methane is numerically investigated using an unstructured, implicit, fully coupled finite volume approach. The non-linear system of equations is solved by Newton's method. The catalytic partial oxidation of methane over rhodium catalyst in a coated honeycomb reactor is studied three-dimensionally, and eight gas-phase species (CH_4, CO_2, H_2O, N_2, O_2, CO, OH and H_2) are considered for the simulation. Surface chemistry is modelled by detailed reaction mechanism including 38 heterogeneous reactions with 20 surface-adsorbed species for the Rh catalyst. The numerical results are compared with experimental data and good agreement is observed. Effects of the design variables, which include the inlet velocity, methane/oxygen ratio, catalytic wall temperature, and catalyst loading on the cost functions representing methane conversion and hydrogen production, are numerically investigated. The sensitivity analysis for the reactor is performed using three different approaches: finite difference, direct differentiation and an adjoint method. Two gradient-based design optimization algorithms are utilized to improve the reactor performance.

17/01750 Development of a multiscale microbial kinetics coupled gas transport model for the simulation of biogenic coalbed methane production

Senthamaraikkannan, G. *et al. Fuel*, 2016, 167, 188–198.

This study developed a multiscale model to simulate coalbed methane (CBM) production from reservoirs along with the inclusion of secondary biogenic gas generated by the continued anaerobic breakdown of coal. A two-step gas transport model is derived for this purpose, based on the assumption that coal porosity can be classified into two scales, macropores and micropores. The model assumes laminar gas flow in macropores and diffusive flow in micropores, driven by desorption. Surface diffusion of gas due to the Klinkenberg effect occurring at low permeability and pressure conditions is also considered. The transport model built for gas flow simulation in a 1D radial reservoir is non-dimensionalized and solved using the Levenberg–Marquardt method. The Morris OAT (one-at-a-time) method for global sensitivity analysis is used to identify important gas transport/storage parameters to perform model refinement for history matching of production data from the gas producing phase of Manville wells found in Alberta. The validated transport model is then combined with a suitably modified enzymatic kinetic model for coal bioconversion that was originally developed by us for lab-scale experiments. Finally, parametric investigations revealed that an order of magnitude increase in the methanogenesis rate can significantly improve biogenic gas recovery, and the next most significant parameter is the solubilization rate.

17/01751 Electrocatalysts for the generation of hydrogen, oxygen and synthesis gas

Sapountzi, F. M. *et al. Progress in Energy and Combustion Science*, 2017, 58, 1–35.

Water electrolysis is the most promising method for efficient production of high purity hydrogen (and oxygen), while the required power input for the electrolysis process can be provided by renewable sources (e.g. solar or wind). The thus produced hydrogen can be used either directly as a fuel or as a reducing agent in chemical processes, such as in Fischer–Tropsch synthesis. Water splitting can be realized both at low temperatures (typically below 100 °C) and at high temperatures (steam water electrolysis at 500–1000 °C), while different ionic agents can be electrochemically transferred during the electrolysis process (OH^-, H^+, O^{2-}). Singular requirements apply in each of the electrolysis technologies (alkaline, polymer electrolyte membrane and solid oxide electrolysis) for ensuring high electrocatalytic activity and long-term stability. The aim of the present article is to provide a brief overview on the effect of the nature and structure of the catalyst–electrode materials on the electrolyser's performance. Past findings and recent progress in the development of efficient anode and cathode materials appropriate for large-scale water electrolysis are presented. The current trends, limitations and perspectives for future developments are summarized for the diverse electrolysis technologies of water splitting, while the case of CO_2/H_2O co-electrolysis (for synthesis gas production) is also discussed.

17/01752 Experimental and modeling analyses of scaling criteria for methane hydrate dissociation in sediment by depressurization

Wang, Y. *et al. Applied Energy*, 2016, 181, 299–309.

Three high-pressure reactors with different inner volumes, which are named as the pilot-scale hydrate simulator (PHS), the cubic hydrate simulator (CHS), and the small cubic hydrate simulator (SCHS), are applied for investigating hydrate dissociation by depressurization method. The volume of the PHS, the CHS, and the SCHS are 117.80, 5.80 and 0.73 L, respectively. Meanwhile, the model of scaling criterion for hydrate dissociation by the depressurization method is developed as well. The scaling criteria are verified and modified by the hydrate dissociation experiments with different scales. Finally, the gas production from a field scale hydrate reservoir (FSHR) is predicted by scaling the experimental results using the modified scaling criteria. The results indicate that the ratios of gas production in the depressurizing (DP) stage are similar to the ratios of inner volume, which verify the scaling criteria in the DP stage. However, the scaling criteria for the experiments in the constant-pressure (CP) stages need to be modified by the experimental results. The correction factor is 0.89. By using the modified scaling criteria, the gas production behaviour, the hydrate dissociation process, and the heat transfer process in a larger scale hydrate reservoir can be predicted. The maximum deviations between the calculated value and experimental result are less than 16%, which can be accepted. In the FSHR with the diameter of 50 m and the length of 60 m, the predicted results indicate that $3.74 \times 10^6\,m^3$ of gas are produced in 120 h (5 days) during the DP stage, and $1.94 \times 10^6\,m^3$ of gas are produced in 1.86×10^5 h (7750 days) during the CP stage.

17/01753 Ni/TiO_2 for low temperature steam reforming of methane

Kho, E. T. *et al. Chemical Engineering Science*, 2016, 140, 161–170.

A titanium dioxide-supported nickel (Ni/TiO_2) catalyst was studied for the low temperature steam reforming of methane (SRM). While studies have frequently reported deactivation/inactivity of TiO_2-supported metal catalysts under conventional high temperature methane reforming conditions, it is shown here that by applying activation treatments at a milder temperature of 400 °C, Ni/TiO_2 is able to maintain stable and effective hydrogen production at 500 °C even at a low steam to methane input ratio of 1 : 1. Temperature programmed reduction studies showed that the presence of nickel species with stronger support interaction is crucial for the low temperature activation of methane while more weakly interacting nickel species contributed to hydrogen production via the water gas shift reaction. This observation was further confirmed when an identical reaction was performed with nickel supported on an inert oxide (silica) whereby the nickel species predominantly possessed a weaker metal–support interaction. When the amount of steam fed into the SRM system was increased, an enhancement in methane conversion by Ni/TiO_2 was observed with up to 45% methane conversion achieved at 500 °C for a

H_2O/CH_4 feed ratio of three. The Ni/TiO_2 catalyst was shown to be capable of maintaining stable conversions and product selectivities for at least 96 h, depending on the H_2O/CH_4 feed ratio.

17/01754 On the selectivity to higher hydrocarbons in Co-based Fischer–Tropsch synthesis

Rytter, E. *et al. Catalysis Today*, 2016, 261, 3–16.

Impact of process variables on selectivity to C_{5+} products during cobalt Fischer–Tropsch synthesis (FTS) are summarized and discussed, comprising temperature; pressure; synthesis gas composition; transport limitations of synthesis gas and products; conversion of CO; and effect of water. Further, effect of catalyst formulation, preparation and activation is included, specifically catalyst synthesis; cobalt crystallite size; crystal structure of cobalt; distribution of crystallites; support materials; pore structure; acidity; surface modifications; reduction and pretreatment. Other topics comprise promoters with focus on reduction promoters including rhenium and nickel; impurities like alkali and sulfur; deactivation and regeneration. Discussion is based on mechanistic understanding, specifically kinetics based on hydrogen assisted CO dissociation; a linear relationship between CH_4 and C_{5+} products; possible reinsertion of olefins; hydrogenation of olefins; and surface coverage based on SSITKA data. It is concluded that the majority of reported data on FTS can be rationalized in terms of a CH_x pool mechanism on cobalt where x shifts toward monomers and high polymerization probability (α-value); or methane and light products formation, depending on synthesis conditions and catalyst properties. Selectivity responses are illustrated mainly based on cobalt catalysts on transition alumina supports. How the support in itself affects C_{5+} selectivity is challenging. There clearly is a change in the composition of the cobalt surface pool of reaction intermediates, but how this change originates in support properties remains to be illuminated. So far there is no direct evidence for the termination process; β-hydrogen abstraction, to play a major role in determining FTS selectivity.

17/01755 Radiative heat release from premixed oxy-syngas and oxy-methane flames

de la Torre, M. *et al. Fuel*, 2016, 166, 567–573.

The abundant supply of coal globally and its energy content per unit mass make the use of this fuel an attractive option for power generation. However, with increasingly strict environmental regulations imposed on greenhouse gas emission technologies the future use of coal in its current form is questionable. One solution to reduce pollutant emissions is oxy-combustion with coal-derived syngas, which can provide a method of using coal efficiently with carbon capture. This paper presents a study of the radiative heat release properties from oxy-syngas and oxy-methane flames. This is relevant since the radiative properties of prospective oxy-combustion systems are not fully known. In many oxy-fuel systems the flue gas stream is recycled and premixed with the fuel and oxidizer to reduce flame temperatures. It is estimated that the radiative heat transfer from these recirculated gases will significantly increase due to the increased emission of radiation from CO_2 and H_2O in the 1.2–5 μm wavelength range, which can impact future combustor design models. Motivated by this, this work aims to provide a study of the global and spectral radiation properties of oxy-syngas combustion and how relevant variables affect radiative emissions. Theses variables include the effect of CO_2 acting as a diluent, percentage of H_2 in the fuel, firing input, and the effects of equivalence ratio on the flame's radiative heat release and spectral radiation of CO_2 and H_2O. The current study reveals that the radiative heat release factor of syngas flames decreases at higher firing inputs. It was also observed that the radiative heat factor decreased at high hydrogen concentrations. An increase in heat release factor is also measured at higher recirculation ratios of CO_2.

17/01756 Scheduling of cracking production process with feedstocks and energy constraints

Su, L. *et al. Computers & Chemical Engineering*, 2016, 94, 92–103.

This paper addresses the short-term scheduling problem for the ethylene cracking process with feedstocks and energy constraints. The cracking production of ethylene is a process with units that have decaying performance, requiring periodic clean-up to restore their performance. Under the condition of limited feedstocks, the production operating mode of the cracking furnaces is to keep yields constant by continuously increasing the coil temperature. The authors present a hybrid MINLP/GDP formulation based on continuous-time representation for the scheduling problem over a finite time horizon. In order to solve the proposed model, which is reformulated as an MINLP model, an improved outer approximation algorithm with multi-generation cuts and problem-dependent integer cuts are developed to solve real large-scale problems. Numerical examples are presented to illustrate the application of the model. Based on analysing the optimal solution and sensitivity of the model, some conclusions are obtained to provide useful suggestions for real cracking process production.

17/01757 Syngas evolutionary behavior during chicken manure pyrolysis and air gasification

Burra, K. G. *et al. Applied Energy*, 2016, 181, 408–415.

The evolutionary behaviour of syngas composition during the pyrolysis and gasification of chicken manure was examined at different temperatures and O_2 concentrations. A gas chromatography was used to quantify the syngas evolved. Pure nitrogen was used for pyrolysis while two different oxygen concentrations (21% and 10%) in nitrogen were used for gasification. Five specific temperatures examined during pyrolysis and gasification were from 600 to 1000 °C in steps of 100 °C. Higher O_2 concentration (21%) produced higher energy yields compared to lower O_2 concentrations. Initial 8–10 min yield produced CO_2 dominant syngas from decarboxylation after which the compositions changed to equilibrium. High temperature and low O_2 concentrations yielded higher CO flow rates and amounts. Equilibrium H_2 content was reduced with an increase in O_2 concentration due to the rapid oxidation of H_2 in the presence of oxidative environment. CH_4 was obtained from thermal cracking with its evolution being similar to that of other higher hydrocarbons evolved, albeit in smaller concentration.

LNG

17/01758 Economic evaluation of a new small-scale LNG supply chain using liquid nitrogen for natural-gas liquefaction

Kim, J. *et al. Applied Energy*, 2016, 182, 154–163.

This study proposed a new liquefied natural gas (LNG) supply chain using liquid nitrogen (LN_2) to liquefy natural gas on a small scale, and analysed the life cycle cost (LCC) and the life cycle profit (LCP) for the supply chain. Natural gas was liquefied with the latent heat of LN_2 without any turbo-machines. The LNG was transported to an LN_2 production site, where LN_2 was produced with the cold (cryogenic) energy of the LNG. Then, LN_2 was transferred to the LNG production site again, completing the cycle. To verify the economics of this supply chain, the LCC and LCP were estimated with different design and operation conditions. This supply chain was found to be significantly profitable because it efficiently used the cold energy of both LNG and LN_2, eliminating the required cost for the regasification process. The results of LCC and LCP showed that the profit of the supply chain was maximized when the pressure of the LNG product was approximately 7 bar, irrespective of the transportation distance. This was because the latent heat and density of LNG were different from those of LN_2. The distance between the LNG and LN_2 production sites was the dominant parameter that governed the economics of this supply chain.

17/01759 Numerical investigation of supercritical LNG convective heat transfer in a horizontal serpentine tube

Han, C.-L. *et al. Cryogenics*, 2016, 78, 1–13.

The submerged combustion vaporizer (SCV) is indispensable general equipment for liquefied natural gas (LNG) receiving terminals. In this paper, numerical simulation was conducted to get insight into the flow and heat transfer characteristics of supercritical LNG on the tube-side of SCV. The SST model with enhanced wall treatment method was utilized to handle the coupled wall-to-LNG heat transfer. The thermal–physical properties of LNG under supercritical pressure were used for this study. After the validation of model and method, the effects of mass flux, outer wall temperature and inlet pressure on the heat transfer behaviours were discussed in detail. Then the non-uniformity heat transfer mechanism of supercritical LNG and effect of natural convection due to buoyancy change in the tube was discussed based on the numerical results. Moreover, different flow and heat transfer characteristics inside the bend tube sections were also analysed. The obtained numerical results showed that the local surface heat transfer coefficient attained its peak value when the bulk LNG temperature approached the so-called pseudo-critical temperature. Higher mass flux could eliminate the heat transfer deteriorations due to the increase of turbulent diffusion. An increase of outer wall temperature had a significant influence on diminishing heat transfer ability of LNG. The maximum surface heat transfer coefficient strongly depended on inlet pressure. Bend tube sections could enhance the heat transfer due to secondary flow phenomenon. Furthermore, based on the current simulation results, a new dimensionless, semi-theoretical empirical correlation was developed for supercritical LNG convective heat transfer in a horizontal serpentine tube. The paper provided the mechanism of heat transfer for the design of high-efficiency SCV.

17/01760 Trade with endogenous transportation costs: the case of liquefied natural gas

Oglend, A. *et al. Energy Economics*, 2016, 59, 138–148.

This paper investigates the relationship between liquefied natural gas (LNG) shipping costs and regional natural gas price spreads. The authors use data on natural gas prices and shipping costs to analyse the distribution of trade benefits within the LNG value chain when shipping costs are endogenous to price spread developments. The empirical analysis suggests that for the 2006–2014 period, the LNG shipping sector has had an implied scarcity rent on LNG shipping capacity of $0.14/MMBtu for the EU/US spread, $0.32/MMBtu for the Asia/EU spread, and $0.42/MMBtu for the Asia/US spread. The authors highlight in a counter-factual analysis that this distributional effect is not economically negligible. They investigate how including endogenous transportation costs affects the measured degree of price convergence between regional natural gas markets. It is found that price convergence is stronger when the authors controlled for variations in transportation costs rather than implicitly assuming fixed or exogenous costs.

Hydrogen generation and storage

17/01761 CFD study on Taconis thermoacoustic oscillation with cryogenic hydrogen as working gas

Sun, D. *et al. Cryogenics*, 2016, 75, 38–46.

Taconis oscillation is a kind of typical self-excited thermoacoustic oscillation, the study of which is of great significance to reveal the thermoacoustic conversion effect and find ways to suppress self-excited oscillation in cryogenic systems. Based on computational fluid dynamics (CFD) method, the onset process of Taconis oscillation with low temperature hydrogen at atmospheric pressure as working gas is first simulated. It is shown that a standing-wave acoustic field operating at 91 Hz starts spontaneously and finally develops to a saturation state in the Taconis tube with length and inner diameter of 1 m and 0.01 m, respectively. Parametric variations in both axial and radial directions of thermoacoustic field are then studied in detail. By combining the computational results with Rott's theory, the spatial distributions of viscous dissipation, thermal relaxation dissipation, and source/sink terms of Taconis thermoacoustic oscillation are obtained quantitatively. The dissipation and source terms are found to be mainly brought forth by the travelling-wave and standing-wave components of the acoustic field, respectively.

17/01762 Comparing hydrogen sorption in different Pd-doped pristine and surface-modified nanoporous carbons

Giasafaki, D. *et al. Carbon*, 2016, 98, 1–14.

Three types of nanoporous carbons (a molecular sieve, an ordered mesoporous carbon and a carbon aerogel) with distinctively different porous properties were subjected to surface modification through wet oxidation and subsequent metal doping with Pd nanoparticles. The H_2 sorption performance of the carbons and their doped analogues was examined at 298 K up to 20 bar. The introduction of different oxygen containing groups in the three carbons enhances the amount of sorbed hydrogen, while the rather complex mechanism of sorption seems to be positively influenced by the small size of the pores and the surface chemistry. It was shown that in all cases a synergistic effect between the metal and the oxidized carbon takes place, leading to enhanced hydrogen sorption through reversible processes, which however is not sufficient to meet the demanding targets for practical applications.

17/01763 Demonstrating hydrogen production from ammonia using lithium imide – powering a small proton exchange membrane fuel cell

Hunter, H. M. A. *et al. Journal of Power Sources*, 2016, 329, 138–147.

Accessing the intrinsic hydrogen content within ammonia, NH_3, has the potential to play a very significant role in the future of a CO_2-free sustainable energy supply. Inexpensive light metal imides and amides are effective at decomposing ammonia to hydrogen and nitrogen ($2NH_3 \rightarrow 3H_2 + N_2$), at modest temperatures, and thus represent a low-cost approach to on-demand hydrogen production. Building on this discovery, this paper describes the integration of an ammonia cracking unit with a post-reactor gas purification system and a small-scale proton exchange membrane fuel cell to create a first bench-top demonstrator for the production of hydrogen using light metal imides.

17/01764 Effects of plate electrode materials on hydrogen production by pulsed discharge in ethanol solution

Xin, Y. *et al. Applied Energy*, 2016, 181, 75–82.

Hydrogen production from an ethanol solution by pulsed high voltage spark discharge was optimized by varying the material of plate electrode. It is the first time that metal work function has been used in hydrogen production by plasma reforming. With low work function metal plate electrode, both energy efficiency and hydrogen yield can be increased. The flow rate and the percentage concentration of hydrogen were achieved 1.3 L/min and 75%, respectively, while discharging with zinc plate electrode for hydrogen production, which is much better than traditional stainless steel electrodes at the same conditions. The analysis of emission spectra was also accomplished in this work. All the intensity of existing spectral lines showed a decline with higher work function metal as plate electrode, and H^+ may be the key to the process of hydrogen production. Additionally, electron temperature and density were also estimated. Both of which were increased with lower work function metal plate electrodes. The electron temperature and density can reach 24,000 K, $7.5 \times 10^{18}\,cm^{-3}$, respectively.

17/01765 Enhanced hydrogen production by sorption-enhanced steam reforming from glycerol with in-situ CO_2 removal in a fixed-bed reactor

Dou, B. *et al. Fuel*, 2016, 166, 340–346.

For the fixed-bed reactor configuration in the sorption-enhanced steam reforming process (SERP), solid mixture of catalyst and sorbent is stationary and alternatively exposed to reaction and regeneration conditions for multi-cycles by periodically switching the feed gases for enhanced hydrogen production with *in situ* CO_2 removal. A NiO/$NiAl_2O_4$ catalyst was synthesized by the co-precipitation method with rising pH technique and the crystalline spinel phase of $NiAl_2O_4$ was formed under the calcination temperature of 900 °C. The catalyst was characterized by X-ray powder diffraction, scanning electron microscope, thermogravimetric analysis and N_2 adsorption–desorption. The non-stoichiometric thermodynamic calculation was carried out to determine the effects of temperature and *in situ* CO_2 removal on the enhancement of hydrogen production by SERP from glycerol at 425–700 °C. The multi-cycles on reaction and regeneration for hydrogen production by SERP from glycerol were performed by NiO/$NiAl_2O_4$ catalyst and CaO based sorbent in a fixed-bed reactor. The results showed that hydrogen production by SERP can be clearly divided into three periods, and the experimental gaseous products were compared with non-stoichiometric thermodynamic calculations. It is obvious that H_2 purity was greatly increased, and CO_2, CO and CH_4 concentrations were reduced by *in situ* CO_2 removal during the pre-breakthrough period. It is found that enhanced hydrogen production was mainly depended on *in situ* CO_2 removal. The operation durations for producing high-purity hydrogen of more than 90% were decreased with the increase of the cycles. It may due to the decrease in the reactivity of CaO based sorbent after multi-cycles reaction and regeneration.

17/01766 Galvanic exchange at layered doubled hydroxide/N-doped graphene as an *in-situ* method to fabricate powerful electrocatalysts for hydrogen evolution reaction

Ensafi, A. A. *et al. Energy*, 2016, 116, 1087–1096.

Introducing a novel strategy for growing dispersed metal nanoparticles at reduced graphene oxide (rGO) and nitrogen-doped GO (rNGO), this work aimed to design Pt-free electrocatalysts for water splitting. For this purpose, gold nanoparticles were fabricated by the *in situ* galvanic exchange of layered double hydroxide (LDH) metals on rGO and rNGO. The significant roles of the galvanic exchange method, LaNi-LDH, and the Au nanoparticles synthesized on the rGO/rNGO-LaNi-LDH surface ($Au^{@}$rGO/rNGO-LaNi-LDH) were investigated via a variety of methods and certain novel properties such as nitrogen–metal bridge bonds between the metal component of $Au^{@}$LDH and the nitrogen component of rNGO were established, which indicated the semi-nanorod morphology of the $Au^{@}$rGO/rNGO-LaNi-LDH thus produced. Electrochemical studies were used to reveal an onset potential of only −80 mV vs RHE at an exchange current density of about $10\,mA\,cm^{-2}$ with a small Tafel slope of $60\,mV\,dec^{-1}$ for the hydrogen generation reaction in a $0.5\,mol\,L^{-1}$ H_2SO_4 solution. The isolated island architecture of rNGO/LaNi-LDH and rNGO/$Au^{@}$LaNi-LDH were found to promise rich and active sites to be exposed, which allow for the effective interaction of the reactants (e.g. protons) with these active sites.

17/01767 Gold supported on zirconia polymorphs for hydrogen generation from formic acid in base-free aqueous medium

Bi, Q.-Y. *et al. Journal of Power Sources*, 2016, 328, 463–471.

Formic acid (FA) has attracted considerable attention as a safe and convenient hydrogen storage material for renewable energy transformation. However, development of an efficient heterogeneous catalyst for selective FA decomposition for ultraclean H_2 gas in the absence of any alkalis or additives under mild conditions remains a major challenge. Based on their previous work on Au/ZrO_2 as a robust and efficient catalyst for FA dehydrogenation in amine system, the authors report here ZrO_2 with different nanocrystal polymorphs supported Au nanoparticles can achieve near completion of FA dehydrogenation in base-free aqueous medium. Of significant importance is that an excellent rate of up to $81.8\,L\,H_2\,g_{Au}^{-1}\,h^{-1}$ in open system and highly pressurized gas of 5.9 MPa in closed one can be readily attained at

80 °C for Au/*m*-ZrO_2. *In situ* diffuse reflectance infrared Fourier transform (DRIFT) and CO_2-temperature programmed desorption (TPD) techniques revealed that Au/*m*-ZrO_2 exhibits a higher density of surface basic sites than Au/*t*-ZrO_2 and Au/*a*-ZrO_2. Basic sites in surface can substantially facilitate crucial FA deprotonation process which appears to be a key factor for achieving high dehydrogenation activity. The H/D exchange between solvent of H_2O and substrate of FA was observed by the kinetic isotope effect experiments.

17/01768 High temperature hydrogen production: design of a 750 KW demonstration plant for a two step thermochemical cycle

Säck, J.-P. *et al. Solar Energy*, 2016, 135, 232–241.

This paper describes the study of a solar reactor for a two-step solar thermo-chemical water splitting cycle concerning the EU-project Hydrosol Plant, which aims to build a plant at the end of 2016 on a solar tower at the Plataforma Solar de Almería with a thermal input power of 750 kW to produce 3 kg/week of hydrogen. The process applies nickel-ferrite as reactive species, which works optimally at 1100 °C for the water splitting step and at 1400 °C for the regeneration step. This material is provided in form of monoliths which are used in cars as catalytic converter. On the platform three reactors are placed to reach a volume of about 0.3 m^3 of active material inside the reactor chambers. During the operations two of these will be regenerated while one will work on water splitting, to reach a quasi-continuous hydrogen production. The design concept of the reactor is taken from the SOLREF reactor, which was originally developed by DLR for methane reforming at 900 °C and 10 bar. The scheme and the layout of the plant to feed the reactors have been studied, too. A thermodynamic model for the regeneration step has been also developed to check if the thermal power demand of the three reactors can be supplied by the defined thermal input power. The differences to the other HYDROSOL projects are: the upscaling from 100 kW to 750 kW, the usage of monoliths completely made of nickel-ferrite and the control strategy with three reactors instead of two.

17/01769 Performance evaluation at different process parameters of an innovative prototype of biomass gasification system aimed to hydrogen production

Pallozzi, V. *et al. Energy Conversion and Management*, 2016, 130, 34–43.

Gasification is currently considered one of the most effective technologies to produce power and hydrogen from biomass and the scope of this work is to determine performances of such an energy system in terms of production of pure hydrogen. The overall plant has been simulated by means of ChemCAD software. It is composed of a dual fluidized bed biomass gasifier with catalytic filter candles (CF), innovatively integrated within the gasification reactor, water gas shift reactor (WGS), equipped with a desulfurization reactor (DeS), and pressure swing adsorber system (PSA), coupled with a micro gas-turbine system (mGT) as an auxiliary power generator aimed to supply inner needs of electricity. Research and pilot scale tests on gasifier, CF, WGS reactor and PSA unit allowed to validate the model. The components have been integrated in a relatively small size and innovative plant (1 MW_{th} as biomass input). This integration entails highly pure H_2 and major efficiency. The model allowed a sensitivity analysis of basic parameters as WGS temperature, residence time and steam to biomass ratio (SB). Important results have been generated reaching a maximum hydrogen yield of 75.2 g_{H2}/kg_{bio} and a maximum efficiency, HHV based, of 55.1%. Optimal compromise of results was obtained with SB equal to 2, WGS reactor temperature at 300 °C and residence time at 0.8 s. Finally, even the chance to generate hydrogen without consumption of auxiliary fuel (by exploiting off gas and waste heat recovery) has been investigated.

17/01770 Pyrolysis of de-oiled seed cake of *Jatropha curcas* and catalytic steam reforming of pyrolytic bio-oil to hydrogen

Renny, A. *et al. Bioresource Technology*, 2016, 220, 151–160.

The aim of this work was to study the pyrolysis of de-oiled seed cake of *Jatropha curcas* and catalytic steam reforming of pyrolytic bio-oil to hydrogen. As per the literature, the presence of heavy nitrogenous and oxygenated compounds leads to catalyst deactivation. Here, an attempt has been made to tune pyrolytic reactions to optimize the N and O content of the pyrolytic bio-oil. Bio-oil conversion and hydrogen yield decreased as reaction progressed, which attributes to temporary loss of catalytic activity by blockage of catalyst pores by carbon deposition. Further, retention of steam reforming activity after repetitive steam activation suggests long-term catalyst usage.

17/01771 System development for solar energy-based hydrogen production and on-site combustion in HCCI engine for power generation

Islam, S. *et al. Solar Energy*, 2016, 136, 65–77.

A solar energy based multigeneration system including hydrogen production and its on-site utilization in homogeneous charge compression ignition (HCCI) engine is developed and analysed energetically and exergetically. This unique design of power generation through on-site utilization of hydrogen minimizes the high costs associated with the transportation and space storage of hydrogen. The exhaust of HCCI engine is used to run an organic Rankine cycle (ORC) turbine and the heat rejected from the ORC working fluid at the exit of turbine is further used to operate an absorption chiller to cool photovoltaic (PV) panels. The operating conditions and their influence on energy and exergy efficiency of overall system and PV panels, and output power of HCCI engine are examined. This innovative cooling system greatly improves the energy and exergy efficiencies of PV panels from 14.9% and 15.7% to 20.7% and 21.8%, respectively. The energy and exergy efficiencies of the overall system are improved significantly, from 37.4% and 33.6% to 53.4% and 46.8%, respectively, after incorporating ORC turbine and absorption chiller. The maximum power generation by the HCCI engine is found to be in the order of 4800 kW. This proposed system appears to be superior to conventional solar-based hydrogen production systems.

17/01772 The impact of furfural concentrations and substrate-to-biomass ratios on biological hydrogen production from synthetic lignocellulosic hydrolysate using mesophilic anaerobic digester sludge

Akobi, C. *et al. Bioresource Technology*, 2016, 221, 598–606.

This study evaluated the impact of furfural (a furan derivative) on hydrogen production rates and yields at initial substrate-to-microorganism ratios ($S°/X°$) of 4, 2, 1 and 0.5 gCOD/gVSS and furfural concentrations of 4, 2, 1 and 0.5 g/L. Fermentation studies were carried out in batches using synthetic lignocellulosic hydrolysate as substrate and mesophilic anaerobic digester sludge as seed. Contrary to other literature studies where furfural was inhibitory, this study showed that furfural concentrations of up to 1 g/L enhanced hydrogen production with yields as high as 19% from the control (batch without furfural). Plots of hydrogen yields against g furfural/g sugars and hydrogen yields versus g furfural/g biomass showed negative linear correlation indicating that these parameters influence biohydrogen production. Regression analysis indicated that g furfural/g $sugars_{initial}$ exerted a greater effect on the degree of inhibition of hydrogen production than g furfural/g VSS_{final}.

04 BY-PRODUCTS RELATED TO FUELS

17/01773 An inverse method to estimate adsorption kinetics of light hydrocarbons on activated carbon

Rahideh, H. *et al. Computers & Chemical Engineering*, 2016, 93, 197–211.

An inverse algorithm to estimate the adsorption kinetics inside the spherical particles in a constant molar flow gas adsorber reservoir by measuring the bulk pressure is developed. The formulation includes Knudsen diffusion, surface diffusion, slip and viscous flows. To obtain an efficient algorithm, the conjugate gradient method for optimization procedure and the incremental differential quadrature method for solving the governing equations are adopted. The results show that the Knudsen diffusion, surface diffusion, slip and viscous flows effects depend on the type of adsorbate and adsorbent gases. It is shown that the effective diffusivity is not constant and goes through a minimum at an intermediate pressure. Also, it is found that the Knudsen diffusion and the viscous flow are the dominant parts of the mass transfer process at low and high pressure, respectively, and despite the viscous flow, the Knudsen diffusion is highly sensitive to temperature change.

17/01774 Evaluation of co-pyrolysis petrochemical wastewater sludge with lignite in a thermogravimetric analyser and a packed-bed reactor: pyrolysis characteristics, kinetics, and products analysis

Mu, L. *et al. Bioresource Technology*, 2016, 221, 147–156.

Co-pyrolysis characteristics of petrochemical wastewater sludge and Huolinhe lignite were investigated using thermogravimetric analyser and packed-bed reactor coupled with Fourier transform infrared spectrometer and gas chromatography. The pyrolysis characteristics of the blends at various sludge blending ratios were compared with those of the individual materials. Thermogravimetric experiments showed that the interactions between the blends were beneficial to generate more residues. In packed-bed reactor, synergetic effects promoted the release of gas products and left less liquid and solid products than those calculated by additive manner. Fourier transform infrared spectrometer analysis showed that main functional groups in chars gradually

disappeared with pyrolysis temperatures increasing, and H_2O, CH_4, CO, and CO_2 appeared in volatiles during pyrolysis. Gas compositions analysis indicated that, the yields of H_2 and CO clearly increased as the pyrolysis temperature and sludge blending ratio increasing, while the changes of CH_4 and CO_2 yields were relatively complex.

17/01775 Homogeneous mercury oxidation with bromine species released from HBr-modified fly ash

Gu, Y. *et al. Fuel*, 2016, 169, 58–67.

This research studies the release of bromine species from HBr-modified fly ash and the subsequent homogeneous oxidation of gaseous elemental mercury (Hg^0) by active gaseous bromine species during heating. Tests utilize an innovative bench-scale experimental system specialized for the homogeneous Hg^0 oxidation reaction and confirm that the released bromine species from the fly ash can oxidize Hg^0 in the gas-phase. Low reaction temperatures are believed to favour the formation of intermediate products and effectiveness of Van der Waals forces resulting in improved mercury oxidation efficiency. Higher reactant concentrations improved oxidation performance, most likely because the oxidation reaction occurs via multiple reaction steps. Furthermore, O_2 may not facilitate the Hg^0 oxidation at the specified reaction temperature. Both FT-IR and UV/vis confirmed the release of HBr and Br_2 from brominated fly ash. TG/MS results provided additional evidence of thermal stability and the identity of the released materials. At 140 °C, HBr was detected by both FT-IR and TG-MS. UV/Vis detected increasing Br_2 levels with increased heating temperature (especially above 200 °C). The suggested mechanism is that the hydrogen atom of the released HBr is attracted to the lattice oxygen, forming active bromine species, such as Br*. The Br* can then recombine to form Br_2, which desorbs at higher temperatures and improves homogeneous Hg^0 oxidation.

17/01776 Measurements and CFD modeling of a pulverized coal flame with emphasis on ash deposition

Beckmann, A. M. *et al. Fuel*, 2016, 167, 168–179.

Measurements of fly ash deposition in a 15 kW pulverized coal jet flame and computational fluid dynamics (CFD)-based mathematical modelling have been performed. The deposits have been collected at two ports at particle Stokes numbers in the 0.02–0.34 range and particle kinetic energies not larger than 2×10^{-9} J. Inertial impaction and thermophoresis have been identified as main mechanisms of particle transport towards the deposition surfaces. Deposition rates on air-cooled probes (600–700 °C surface temperature) have been measured to be 24% (Port 2) and 79.4% (Port 3) larger than those measured on uncooled probes (1150 °C surface temperature) due to the enhanced role of thermophoresis. Complex dependencies of the deposition rate on the probe surface temperature and the probe location have been observed. The CFD-model predictions are able to reproduce these dependencies after adjustments to the particle sticking sub-model. The paper contains estimations of both the impaction and sticking efficiencies.

17/01777 Natural sisal fibers derived hierarchical porous activated carbon as capacitive material in lithium ion capacitor

Yang, Z. *et al. Journal of Power Sources*, 2016, 329, 339–346.

The lithium-ion capacitor (LIC) is a novel advanced electrochemical energy storage (EES) system bridging gap between lithium ion battery (LIB) and electrochemical capacitor (ECC). This study reports that sisal fibre activated carbon (SFAC) was synthesized by hydrothermal treatment followed by KOH activation and served as capacitive material in LIC for the first time. Different particle structure, morphology, specific surface area and heteroatoms affected the electrochemical performance of as-prepared materials and corresponding LICs. When the mass ratio of KOH to char precursor was 2, hierarchical porous structured SFAC-2 was prepared and exhibited moderate specific capacitance (103 F g^{-1} at 0.1 A g^{-1}), superior rate capability and cyclic stability (88% capacity retention after 5000 cycles at 1 A g^{-1}). The corresponding assembled LIC (LIC-SC2) with optimal comprehensive electrochemical performance, displayed the energy density of 83 Wh kg^{-1}, the power density of 5718 W kg^{-1} and superior cyclic stability (92% energy density retention after 1000 cycles at 0.5 A g^{-1}). It is worthwhile that the source for activated carbon is a natural and renewable one and the synthesis method is eco-friendly, which facilitate that hierarchical porous activated carbon has potential applications in the field of LIC and other energy storage systems.

17/01778 Observation of vertical variability of black carbon concentration in lower troposphere on campaigns in Poland

Chilinski, M. T. *et al. Atmospheric Environment*, 2016, 137, 155–170.

This study presents two methods for observation of black carbon (BC) vertical profiles in lower troposphere based on the micro-aethalometer AE-51. In the first method a micro-aethalometer was carried by the observer along a trail on the slope of the mountain valley. The second method used an unmanned aerial vehicle as a platform for collecting data up to 1500 m above ground. This study presents vertical profiles collected in and above the Subcarphatian Wislok valley. Profiles measured as part of the trial on the slopes of Wislok valley, were collected during strong smog conditions during the autumn/winter season, when BC concentration reached values above 60 μg/m^3. The smog intensive layer is often close to the surface (up to 100 m) as a results of surface inversion and the mountain breeze circulation, which during the night transports air pollution emitted from houses toward the valley's bottom. Usually the vertical profiles of BC concentration show significant reduction with the altitude, however, some multi-layered structures were also observed during night time inversion conditions. It was found that smog condition can develop in clean air mass, and in those cases local pollution has significant impact on the columnar aerosol properties. During such conditions the aerosol optical depth shows a diurnal cycle not observed in the long-term data. The UAV flights in the lower troposphere were conducted during two sessions, one with clean polar air masses (BC concentration < 1 μg/m^3) and second with moderate aerosol conditions (BC concentration 1–5 μg/m^3). The profile of BC concentration shows stratification of absorbing aerosols in a shape of multi-layer structures similar to the lidar/ceilometer signals.

17/01779 Oxidation effects on in-plane and interlaminar shear strengths of two-dimensional carbon fiber reinforced silicon carbide composites

Zhang, Y. *et al. Carbon*, 2016, 98, 144–156.

Effects of oxidation on in-plane shear strength and interlaminar shear strength of two-dimensional carbon fibre reinforced silicon carbide composites (2D C/SiC) were studied based on the corresponding shear damage mechanisms. The results showed that oxidation had resulted in severe degradations of the two strengths, however, it had little influence on the shear failure mechanisms. Under in-plane shear loading, large-scale fibre bridging mechanism controlled the shear behaviours. A modified rigid body sliding model was proposed to characterize the in-plane shear strength. In comparison, interface sliding mechanism controlled the interlaminar shear strength. Based on above failure mechanisms, the two shear strengths were quantitatively characterized by the constituent properties, such as diameter of carbon fibres, interface sliding stress, matrix fracture energy and matrix cracking spacing. Therefore, oxidation effects on them were attributed to the decreased constituent properties which mainly results from oxidation consumption of the carbon phases. Finally, for the conditions of this study, a relationship was proposed that the interlaminar shear strength equals the in-plane shear strength minus the fibre bridging stress.

17/01780 Proposal of a new soot quantification method and investigation of soot formation behavior in coal gasification

Umemoto, S. *et al. Fuel*, 2016, 167, 280–287.

Coal gasification is one of the key technologies for utilization of coal. Coal gasification mainly consists of coal pyrolysis, char gasification, and gas-phase reactions. Soot is made up of fine solid carbon particles formed by volatile matter decomposition and has lower gasification reactivity than char. Since the solid products of coal gasification contain both char and soot, it is difficult to quantify the amount of soot produced by this process. In this study, a novel soot and char quantification method utilizing a laser diffraction particle size analyser is proposed. Coal gasification experiments were performed using a pressurized drop tube furnace. The soot and char yields were quantified by the new method. During CO_2 gasification, char was selectively gasified and the amount of soot barely decreased. Hence, the carbon conversion initially increased, but remained around 0.8 even at 1673 K. In the case of other gasifying agents, O_2 or H_2O, different behaviour was found. During O_2 gasification, the soot yield considerably decreased as the O_2 concentration increased. The main reason was not soot gasification, as presumed, but rather the reaction of tar components with O_2. In the H_2O gasification, the soot yield slightly decreased as the H_2O concentration increased.

17/01781 Removal of elemental mercury from flue gas by recyclable $CuCl_2$ modified magnetospheres catalyst from fly ash. Part 2. Identification of involved reaction mechanism

Yang, J. *et al. Fuel*, 2016, 167, 366–374.

The Hg^0 adsorption and oxidation sites on the $CuCl_2$-MF catalyst as well as the role of atomic Cu and Cl in Hg^0 removal were identified by a temperature programmed desorption experiment. The reaction mechanism with the participation of O_2 and HCl was investigated. The changes in surface chemistry of fresh, spent and *in situ* pretreated catalyst with O_2 and/or HCl were investigated by EPR and XPS to better understand the intermediate reaction products and steps. The results suggested that different mercury adsorption sites are existed on the catalyst: Cl adsorption sites and Cu adsorption sites. The binding energy of mercury on the Cu adsorption sites is higher than that on the Cl adsorption sites. O_2 and HCl significantly affected the state of Cu and Cl on the spent catalyst. The interaction between Hg^0 and $CuCl_2$ with the participation of O_2 and/or HCl follows three steps mechanism: (1) the reduction of $CuCl_2$ to CuCl for the interaction with Hg^0, (2) the

reoxidation of CuCl for the interaction with O_2 forming an intermediate copper oxygen chloride species, (3) the rechlorination of oxychloride species resulting in the restoration of $CuCl_2$. This demonstrated that the interaction between Hg^0 and $CuCl_2$ is a cycle when O_2 and HCl are contained in the reaction system.

17/01782 Selection of the most influential flow and thermal parameters for predicting the efficiency of activated carbon filters using neuro-fuzzy technique
Raos, M. *et al. Building and Environment*, 2016, 104, 68–75.
This paper analyses the influence of various flow and thermal variables on the performance of the activated carbon filter in the air-conditioning system. The adaptive neuro fuzzy inference system method was applied to the data obtained from the experimental apparatus in order to select the most influential parameters for assessing the efficiency of the activated carbon filter. Acetone was selected as the target pollutant component. Experiments were performed for different temperature, humidity, and flow rate conditions, as well as for acetone concentrations. A set of four potential inputs was considered: velocities of gas mixture through ventilation duct (flow), temperature, humidity, and concentration of test chemical pollutants ahead of the filter module. The results show that the most influential parameter for predicting outlet concentrations of acetone is temperature.

17/01783 Sensitivity study of engine soot forming using detailed soot modelling oriented in soot surface growth dynamic
Zhao, F. *et al. Fuel*, 2016, 168, 81–90.
Development of detailed soot model independent of empirical expression is supposed to reasonably replicate the soot formation and oxidation dynamic kinetics over a wide range of diesel engine operations, thus facilitates exploring crucial factor of soot forming. Based on comprehending of varying mixture inhomogeneity on soot forming under engine operations, a new multi-step soot model oriented in surface growth dynamic had so far been updated in this study. By correlation analysis, the new soot model is able to display the influence of both temperature and mixture inhomogeneity on soot surface activity by revising the parameter of the fraction of active sites. Hence the dominant factor of soot forming is conducted by sensitivity study in aspect of three distinctive phases: fast soot inception, soot growth equilibrium and soot oxidation prevailing, under varying mixture inhomogeneity. The soot inception is more influenced by temperature under uniform mixture combustion, but the dominant factor is switched to mixture inhomogeneity in stratified mixture wherein the acetylene formation rate gets the maximum. Similarly, less oxygen helps soot abatement due to weaker chemistry reactive in soot surface growth caused by lower temperature in homogenous mixture. Nevertheless, stimulated soot surface growth by activated surface activity and vast precursor deposit under heterogeneous mixture conduces to soot forming. Simultaneously, impaired soot surface oxidation under non-uniform mixture accelerates the deteriorated engine-out soot in comparison with discharged soot in less homogenous mixture.

17/01784 The effect of selenite on mercury re-emission in smelting flue gas scrubbing system
Peng, B. *et al. Fuel*, 2016, 168, 7–13.
Recently, the mercury re-emission from the scrubbing solution has become a hot topic in wet flue gas desulfurization process (WFGD). Selenite is one of the most important matters in the solution. It is discovered that selenite have great effect on the mercury re-emission in the WFGD process in this paper. Several important parameters, such as selenite concentration, pH value, temperature and chloride concentration, and reaction mechanisms were studied on the Hg^0 re-emission. The experimental results indicate that mercury reduction and re-emission can be effectively inhibited with high selenite and chloride concentrations, low temperature and pH value. The mechanisms for inhibition of mercury reduction and re-emission are proved to be different under acid and alkaline conditions respectively. Under acid condition, it is the formation of stable HgSe that decrease Hg^0 re-emission. However, the formation of more stable $HgSeO_3SO_3^{2-}$ or $Hg(SeO_3)_2^{2-}$ than $Hg(SO_3)_2^{2-}$ contributes to avoid the oxidized mercury reduction by sulfite ions and then the mercury re-emission under the alkaline condition. In addition, it is also found that Cl^- ions can further enhance the inhibition effect and suppress Hg^0 re-emission by the formation of stable $HgSeO_3Cl^-$ and $HgSeO_3Cl_2^{2-}$ complexes.

17/01785 Unburned carbon from lignite fly ash as an adsorbent for SO_2 removal
Kisiela, A. M. *et al. Energy*, 2016, 116, 1454–1463.
The aim of this work is to investigate the possibility of application of unburned carbon from lignite fly ash for the purpose of SO_2 adsorption from flue gases. The subject of research are three fraction of unburned carbon, which were formed during the nominal operation of Belchatów power station (PGE GiEK) in Poland. In order to characterize the adsorption properties of the investigated materials, a comprehensive research procedure was carried out, including: proximate and ultimate analysis, determination of calorific value, textural characterization (C_6H_6 and CO_2 physisorption, scanning electron microscope), surface chemistry characterization (X-ray diffraction), inductively coupled plasma-optical emission spectrometry, temperature-programmed desorption, point of zero charge), determination of ignition temperature (differential scanning calorimetry, DSC) and SO_2 adsorption tests using a fixed bed of an adsorbent. Conducted analyses show that high carbonaceous wastes, being a result of rapid and intense oxidation of lignite in an industrial boiler, exhibit high potential for adsorption and are characterized by the competitive properties relative to carbon materials, obtained in the laboratory conditions and presented in the literature. It has also been shown, that the chemical nature of adsorbent surface has a significant impact on the effectiveness of SO_2 adsorption and on the adsorbate selectivity. Own research demonstrates, that an increase of sulfur dioxide adsorption is observed with an increase of the oxygen surface groups content, i.e. carboxylic acids and lactones, which formation is favoured in conditions prevailing in the industrial boiler. Own research, dedicated to determination of ignition temperature of unburned carbons, confirmed the validity of application of DSC analysis for this purpose. The research results, presented in this work show, that unburned carbons from lignite fly ash, in particularly UN-B and UN-C, have competitive surface structure properties relative to commercially available activated carbons: AKP-5 and AKP-5/A, and can be successfully used as adsorbents for flue gases desulfurization.

05 NUCLEAR FUELS

Scientific, technical

17/01786 A natural cement analogue study to understand the long-term behaviour of cements in nuclear waste repositories: Maqarin (Jordan)
Martin, L. H. J. *et al. Applied Geochemistry*, 2016, 71, 20–34.
The geological storage of nuclear waste includes multibarrier engineered systems where a large amount of cement-based material is used. Predicting the long term behaviour of cement is approached by reactive transport modelling, where some of the boundary conditions can be defined through studying natural cement analogues (e.g. at the Maqarin natural analogue site). At Maqarin, pyrometamorphism of clay biomicrites and siliceous chalks, caused by the *in situ* combustion of organic matter, produced various clinker minerals. The interaction of infiltrating groundwater with these clinker phases resulted in a portlandite-buffered hyperalkaline leachate plume, which migrated into the adjacent biomicrite host rock, resulting in the precipitation of hydrated cement minerals. In this study, rock samples with different degrees of interaction with the hyperalkaline plume were investigated by various methods (mostly SEM-EDS). The observations have identified a paragenetic sequence of hydrous cement minerals, and reveal how the fractures and porosity in the biomicrite have become sequentially filled. In the alkaline disturbed zone, C–A–S–H (an unstoichiometric gel of Ca, Al, Si and OH) is observed to fill the pores of the biomicrite wallrock, as a consequence of reaction with a high pH Ca-rich fluid circulating in fractures. Porosity profiles indicate that in some cases the pores of the rock adjacent to the fractures became tightly sealed, whereas in the veins some porosity is preserved. Later pulses of sulfate-rich groundwater precipitated ettringite and occasionally thaumasite in the veins, whereas downstream in the lower pH distal regions of the hyperalkaline plume, zeolite was precipitated. Comparing these observations with the reactive transport modelling results reveals two major discrepancies: firstly, the models predict that ettringite is precipitated before C–A–S–H, whereas the C–A–S–H is observed as the earlier phase in Maqarin; and, secondly, the models predict that ettringite acts as the principal pore-filling phase in contrast to the C–A–S–H observed in the natural system. These discrepancies are related to the fact that the data were not available at the time the modelling studies were performed. However, all models succeeded in reproducing the porosity reduction observed at the fracture–rock interface in the natural analogue system.

17/01787 A nonlinear reactivity method with application to accident-tolerant fuels
Roberts, J. A. *et al. Annals of Nuclear Energy*, 2016, 94, 581–588.
A non-linear reactivity model with thermal-hydraulic feedback is presented for analysis of pressurized water reactors fuel with various cladding materials. The simplified, batch-wise neutronic model

requires batch reactivities and migration areas as predetermined functions of burnup, temperature (fuel and coolant), and any design parameters having neutronic significance (e.g. enrichment or cladding composition). Here, such functions are found by using symbolic regression, a unique approach that finds both a functional form and any model coefficients simultaneously. Core thermal-hydraulics are modelled using single-channel, axially-averaged values. The models were implemented in an open-source, Python-based tool, used here to the analyse fuel with Zr-based cladding having outer, protective layers of either FeCrAl or SiC, two materials proposed for use in next-generation, accident-tolerant fuel.

17/01788 Aerial work robot for a nuclear power plant with a pressurized heavy water reactor

Shin, H. *et al. Annals of Nuclear Energy*, 2016, 92, 284–288.

This paper presents an aerial work robot for a nuclear power plant with a pressurized heavy water reactor (PHWR). The aerial work robot provides measurements by teleoperating a fuel handling machine placed at a high location in front of the PHWR. The robot can detect a leak from pipes such as delayed neutron (DN) monitoring tubes, which are also placed at a high place. The robot is equipped with radiation-hardened controllers, radiation-hardened cameras, and a noise robust communication system.

17/01789 An assessment of temperature history on concrete silo dry storage system for CANDU spent fuel

Lee, D.-G. *et al. Annals of Nuclear Energy*, 2016, 94, 263–271.

Concrete silo is a dry storage system for spent fuel generated from CANDU reactors. The silo is designed to remove passively the decay heat from spent fuel, as well as to secure the integrity of spent fuel during storage period. Dominant heat transfer mechanisms must be characterized and validated for the thermal analysis model of the silo, and the temperature history along storage period could be determined by using the validated thermal analysis model. Heat transfer characteristics on the interior and exterior of fuel basket in the silo were assessed to determine the temperature history of silo, which is necessary for evaluating the long-term degradation behaviour of CANDU spent fuel stored in the silo. Also a methodology to evaluate the temperature history during dry storage period was proposed in this study. A computational fluid dynamics (CFD) model of fuel basket including fuel bundles was suggested and temperature difference correlation between fuel bundles and silo's internal member, as a function of decay heat of fuel basket considering natural convection and radiation heat transfer, was deduced. Temperature difference between silo's internal cavity and ambient air was determined by using a concept of thermal resistance, which was validated by CFD analysis. Fuel temperature was expressed as a function of ambient temperature and decay heat of fuel basket in the correlation, and fuel temperature along storage period was determined. Therefore, it could be used to assess the degradation behaviour of spent fuel by applying the degradation mechanism expressed as a function of spent fuel temperature.

17/01790 Analytical solutions to the Stefan problem with internal heat generation

McCord, D. *et al. Applied Thermal Engineering*, 2016, 103, 443–451.

A first-order, ordinary differential equation modelling the Stefan problem (solid–liquid phase change) with internal heat generation in a plane wall is derived and the solutions are compared to the results of a computational fluid dynamics analysis. The internal heat generation term makes the governing equations non-homogeneous so the principle of superposition is used to separate the transient from steady-state portions of the heat equation, which are then solved separately. There is excellent agreement between the solutions to the differential equation and the computational fluid dynamics results for the movement of both the solidification and melting fronts. The solid and liquid temperature profiles show a distinct difference in slope along the interface early in the phase change process. As time increases, the changes in slope decrease and the temperature profiles become parabolic. The system reaches steady-state faster for larger Stefan numbers and inversely, the time to steady-state increases as the Stefan number decreases.

17/01791 Assessment of TASS/SMR code for a loss of coolant flow transient using results of integral type test facility

Chung, Y.-J. *et al. Annals of Nuclear Energy*, 2016, 92, 1–7.

Many countries have taken an interest in small- and medium-sized nuclear power plants. SMART, which was developed by Korea Atomic Energy Research Institute (KAERI), is a small-sized integral type pressurized water reactor with a rated thermal power of 330 MW. In order to analyse thermal hydraulic characteristics of the SMART design, the TASS/SMR code has been developed. The code was validated using the results of basic and separate effect tests including small-scale experiments for the SMART special components. To enhance an analysis capability of the TASS/SMR code for an integral type pressurized water reactors, the KAERI has constructed the VISTA-ITL facility, and several integral effect tests have been performed at the VISTA-ITL facility. The TASS/SMR code is validated using the results of a loss of coolant flow transient, which is one of the integral effect tests performed at the VISTA-ITL. According to the evaluation results, the code predicts well the overall thermal hydraulic behaviours including the system pressure, fluid temperature, and mass flow rate. The main coolant pump model is important in order to simulate well the primary coolant flow behaviour at an early transient.

17/01792 CAD-based hierarchical geometry conversion method for modeling of fission reactor cores

Gan, Q. *et al. Annals of Nuclear Energy*, 2016, 94, 369–375.

The fission reactor core models are usually constructed with abundant nested repeated-structure in several levels. Accordingly, hierarchical descriptions have been adopted in many Monte Carlo (MC) codes to describe fission reactor core efficiently. As the geometry of fission reactor core is more and more complex, modelling for them with some mature computer-aided design (CAD) system becomes more popular. However, the conventional CAD-based MC automatic modelling methods concentrate on decomposing the complex geometries, whereas the hierarchical geometries are neglected. Furthermore, it is time consuming to decompose huge number of geometries in sequence. This paper presents a new method which can generate the hierarchical geometries for MC codes and CAD system in batches. The method can create or gather the hierarchical information as well as other parameters of the models into a dedicated data structure, which can be saved in geometric hierarchy tree (GH-tree). Based on GH-tree, the MC calculation models and CAD models can be generated effectively and accurately. In this paper, the new algorithms were implemented based on the framework of the super Monte Carlo simulation program for nuclear and radiation process (SuperMC), developed by FDS team, and were validated using the models of China Lead-based Research Reactor (CLEAR-I) and IAEA-BN600. The efficiency and accuracy of the new method were demonstrated by the numerical calculation results.

17/01793 CFD simulations on the dynamics of liquid sloshing and its control in a storage tank for spent fuel applications

Sanapala, V. S. *et al. Annals of Nuclear Energy*, 2016, 94, 494–509.

Spent nuclear liquid waste is often kept in partially filled storage tanks. When such storage tanks are subjected to wind and/or earthquake induced excitations, this could lead to detrimental conditions. Therefore, storage tank designers should ensure safe design margins and develop methodologies to overcome a wide range of possible scenarios. In this study, systematic numerical simulations are carried out to investigate the sloshing dynamics of liquid in a storage tank, subjected to seismic excitation. As a precursor, the influence of resonant harmonic excitation on the free surface displacement, pressure distribution, slosh forces, etc. is studied. To suppress the free surface fluctuations and the associated slosh force, two types of baffles viz., ring and vertical baffle are examined. Based on the response to an imposed harmonic excitation, the vertical baffle plate in the middle of the tank, was found to be effective and its dimensions are systematically optimized. This baffle geometry was tested for a well-known seismic excitation (El Centro) and it was observed to effectively suppress free surface fluctuations and the slosh forces.

17/01794 Chemical and Sr isotopic characterization of North America uranium ores: nuclear forensic applications

Balboni, E. *et al. Applied Geochemistry*, 2016, 74, 24–32.

This study reports major, minor, and trace element data and Sr isotope ratios for 11 uranium ore (uraninite, UO_{2+x}) samples and one processed uranium ore concentrate (UOC) from various US deposits. The uraninite investigated represent ores formed via different modes of mineralization (e.g. high- and low-temperature) and within various geological contexts, which include magmatic pegmatites, metamorphic rocks, sandstone-hosted, and roll front deposits. In situ trace element data obtained by laser ablation-ICP-MS and bulk sample Sr isotopic ratios for uraninite samples investigated here indicate distinct signatures that are highly dependent on the mode of mineralization and host rock geology. Relative to their high-temperature counterparts, low-temperature uranium ores record high U/Th ratios (>1000), low total rare earth element (REE) abundances (<1 wt%), high contents (>300 ppm) of first row transition metals (Sc, Ti, V, Cr, Mn, Co, Ni), and radiogenic $^{87}Sr/^{86}Sr$ ratios (>0.7200). Comparison of chondrite normalized REE patterns between uraninite and corresponding processed UOC from the same locality indicates identical patterns at different absolute concentrations. This result ultimately confirms the importance of establishing geochemical signatures of raw, uranium ore materials for attribution purposes in the forensic analysis of intercepted nuclear materials.

17/01795 Delayed neutron detection with graphite moderator for clad failure detection in sodium-cooled fast reactors

Rohée, E. *et al. Annals of Nuclear Energy*, 2016, 92, 440–446.

In order to meet clean core challenges in sodium-cooled fast reactors (SFR), specific attention is paid to the cladding integrity. To monitor this integrity, delayed neutron detection (DND) systems are implemented. During clad failures, neutron precursor fission products (mainly halogens: ^{137}I, ^{87}Br, ^{88}Br) escape into the primary coolant. The detection of these precursors through their delayed neutron emission ensures a diagnosis on clad failures events. In DND systems, ^{3}He proportional counters are selected as the best available technology for neutron detection purposes. Associated with ^{3}He counters, polyethylene blankets are required in order to thermalize neutrons. The first part of this study is dedicated to the optimization of the DND device by Monte-Carlo simulations in order to improve the detection capability. This optimization focuses on the device design presenting a graphite based alternative to polyethylene blankets in order to remove photoneutron noise from $^{2}D(\gamma,n)$ reactions in polyethylene in presence of a high ^{24}Na activity (emission of gamma-rays at 2.75 MeV). The experimental part of this study is devoted to the validation of a measuring station including an ^{3}He counter with carbon for neutron moderation. Both Monte Carlo simulations and experimental results highlight the potential for a low-noise DND system based on graphite moderation.

17/01796 Neutronic and fuel cycle comparison of uranium and thorium as matrix for minor actinides bearing-blankets

Kooyman, T. and Buiron, L. *Annals of Nuclear Energy*, 2016, 92, 61–71.

Minor actinides transmutation is one of the three main axes defined by the 2006 French law for nuclear waste management, along with long-term storage and use of a deep geological repository. In the heterogeneous approach, minor actinides are loaded in specially designed targets assemblies which are located in the periphery of the core, in order to limit the impacts on core operations. This paper compares the use of uranium and thorium dioxide as support matrix in which minor actinides are diluted in the target assemblies. Both UO_2 and ThO_2 exhibit sufficiently good irradiation behaviour to withstand the long residence time associated with heterogeneous transmutation. Five different reprocessing strategies are compared in which some or all the elements in the blankets are reused after reprocessing. The impacts on core safety parameters and fuel cycle parameters are also evaluated for each case and it is found that using thorium as support matrix with reuse of uranium-233 leads to transmutation performances similar to the one obtained with the reuse of plutonium from uranium blankets with slightly lower global impacts on reactor operation and fuel cycle.

17/01797 Occurrence of uranium in Chinese coals and its emissions from coal-fired power plants

Zhang, Y. *et al. Fuel*, 2016, 166, 404–409.

Uranium is a trace elemental in coal. The uranium content from coal mines in China and its distribution in coal-fired power plant effluents was studied and reported in this paper. Chinese coal samples from 18 coal mines were collected and analysed for uranium. It was found that the uranium content for most of the coals was in the range from 1 to 3 mg/kg. Laboratory experiments with a tubular furnace indicate that the amount of uranium released from heated coal increases with temperature and with the retention time, when it combust. Most of the uranium (about 90%) in the coal can be transferred to the ash. Full-scale field tests were carried out at a coal-fired power plant to investigate the uranium distribution (and mass balance) in the coal, limestone, fly ash, bottom ash, gypsum and the flue gas. Almost all the uranium in the coal concentrated in the fly ash (about 80%) and the bottom ash (about 10%). The uranium content in the flue gas was less than 1/1000 of the total elemental input, between 0.043 and 0.069 μg/m^3, which is much lower than the typical concentration of mercury or arsenic in flue gas of coal-fired power plant. The uranium content in the desulfurization gypsum product was found to be slightly larger than the uranium content of the limestone.

17/01798 On the adoption of carbon dioxide thermodynamic cycles for nuclear power conversion: a case study applied to Mochovce 3 nuclear power plant

Santini, L. *et al. Applied Energy*, 2016, 181, 446–463.

In this study, closed CO_2 cycles are investigated for potential application in existing nuclear power stations, referring in particular to the Mochovce power station currently under construction in the Slovak Republic. Three different CO_2 cycles layouts are explored in the range of temperatures offered by the nuclear source and of the existing cooling towers. The investigation shows that the common opinion that S-CO_2 cycles are well suited in the medium to a high temperature range only (higher than about 450 °C) seems unjustified. For a primary heat source with a maximum temperature of 299 °C and a heat sink with a minimum temperature of 19 °C and reasonable assumptions about advanced turbomachines and heat exchanger performances, the supercritical recompressed reheated regenerative CO_2 cycle would yield a net efficiency of 34.04%, which compares well with the 33.51% net efficiency of the existing Rankine cycle. The estimated length of the complete turboset (two turbines, one pump and one compressor) would be less than 11 m (versus two wet steam turbines of 22 m each for the same power), resulting in a factor of 10 reduction in the footprint of the balance of plant. The total CO_2 cycle equipment and main pipelines would have a combined weight of 3957 tons, while in the Mochovce 3 nuclear power plant existing Rankine cycle, the main components and connecting piping weigh nearly 7377 tons, thus a 40% reduction. These results suggest that the adoption of CO_2 in nuclear power stations would not penalize the plant efficiency and would yield significant savings on installation costs and construction times from the much more compact balance of plant.

17/01799 Solid deposition in the ITER cryogenic viscous compressor

Zhang, D. *et al. Cryogenics*, 2016, 78, 14–26.

A transient model for the ITER cryogenic viscous compressor (CVC) is presented. The CVC is designed to separate hydrogen isotopes from helium in the gas-mixture exhaust from the ITER torus. During their residence in the CVC, hydrogen isotopes are captured along the pump wall while helium flows through. The CVC thereby provides the first stage of helium compression. The transient model characterizes the transport phenomena (species, momentum, and energy) that occur in the CVC. The numerical results are compared with experimental data from a scaled down test of the ITER CVC using pure hydrogen. Although the model has been developed for a hydrogen–helium mixture, it is simplified here in order to compare with the experimental data. The transient model, along with other numerical models developed here, provide guidance for the design and optimization of the ITER CVC. The model can also be a useful tool or a reference for similar analyses, such as those for cryogenic carbon capture and air ingress in vacuum isolated cryogenic vessels.

17/01800 Standardized verification of fuel cycle modeling

Feng, B. *et al. Annals of Nuclear Energy*, 2016, 94, 300–312.

A nuclear fuel cycle systems modelling and code-to-code comparison effort was coordinated across multiple national laboratories to verify the tools needed to perform fuel cycle analyses of the transition from a once-through nuclear fuel cycle to a sustainable potential future fuel cycle. For this verification study, a simplified example transition scenario was developed to serve as a test case for the four systems codes involved (DYMOND, VISION, ORION, and MARKAL), each used by a different laboratory participant. In addition, all participants produced spreadsheet solutions for the test case to check all the mass flows and reactor/facility profiles on a year-by-year basis throughout the simulation period. The test case specifications describe a transition from the current US fleet of light water reactors to a future fleet of sodium-cooled fast reactors that continuously recycle transuranic elements as fuel. After several initial coordinated modelling and calculation attempts, it was revealed that most of the differences in code results were not due to different code algorithms or calculation approaches, but due to different interpretations of the input specifications among the analysts. Therefore, the specifications for the test case itself were iteratively updated to remove ambiguity and to help calibrate interpretations. In addition, a few corrections and modifications were made to the codes as well, which led to excellent agreement between all codes and spreadsheets for this test case. Although no fuel cycle transition analysis codes matched the spreadsheet results exactly, all remaining differences in the results were due to fundamental differences in code structure and/or were thoroughly explained. The specifications and example results are provided so that they can be used to verify additional codes in the future for such fuel cycle transition scenarios.

17/01801 Thermodynamic modeling of a nuclear energy based integrated system for hydrogen production and liquefaction

Ozcan, H. and Dincer, I. *Computers & Chemical Engineering*, 2016, 90, 234–246.

A nuclear-based integrated system for hydrogen production and liquefaction with a newly developed four-step magnesium–chlorine cycle is proposed. The system uses nuclear energy to supply heat for the Rankine cycle and Mg–Cl cycle, where the power produced by the Rankine cycle is used to run the electrolysis steps of the Mg–Cl cycle and liquefaction cycle compressors. The four-step Mg–Cl cycle is specifically designed to decrease the electrical work consumption of the cycle by capturing HCl in dry form with an additional step to conventional three-step cycle. A performance assessment study is undertaken based on energy and exergy analysis of the subsystems, and total energy and exergy efficiencies of the plant are found to be 18.6%,

and 31.35%. The comparisons of the subsystem efficiencies and total exergy destructions show that highest irreversibility ratio belongs to the Mg–Cl cycle by 41%, respectively.

17/01802 Thermodynamic performance of pressurized water reactor power conversion cycle combined with fossil-fuel superheater

Wibisono, A. F. and Shwageraus, E. *Energy*, 2016, 117, 190–197.

It is known that the pressurized water reactors (PWRs), which are the most common type of nuclear reactor existing today, usually used to provide a base load electricity. In order to be able to compete with other generation types (fossil and renewables), it would be desirable to develop PWRs with flexible load following capabilities to cope with varying electricity demand, especially in deregulated markets. The thermal efficiency of PWRs can be increased by fitting the power plant with conventional fossil fuel superheaters. This hybrid system has been hypothesized to be able to adjust the power output and the cycle efficiency of PWRs. Such mode of operation would also improve the efficiency of converting the fossil fuel heat because it is applied only at the superheater stage. There are several ways to supply the heat to the superheaters, for example, by using the exhaust gas from the gas turbines and using the conventional gas burner. In this paper, the thermodynamic performance of the hybrid system (PWR with superheater) is investigated for large reactor and small modular reactor (SMR) application. The thermal efficiency of the AP1000 can be improved from 30.2% to 45.8% (with CCGT), 35.6% (with gas burner), and 36.6% (gas burner with reheating). The thermal efficiency of the SMR can be improved from 33.4% to nearly 45% (with CCGT), 35.5% (with gas burner), and 37.4% (gas burner with reheating). The analysis results show that it is possible for the hybrid system to operate between 65% and the full power load.

Economics, policy, supplies, forecasts

17/01803 Advances in the Pennsylvania State University NEM code

Thompson, S. A. and Ivanov, K. N. *Annals of Nuclear Energy*, 2016, 94, 251–262.

The Pennsylvania State University nodal expansion method (NEM) code has been updated in an attempt to enable the code to model more neutronically complex reactor cores, such as those containing mixed-oxide fuel, low leakage cores, and cores that contain multiple burnable poison types. Current nodal methods, which are primarily focused on solving the diffusion equation using a nodal expansion method with the transverse leakage term solved using the quadratic leakage approximation, are known to be inaccurate in such environments. The NEM code is updated with a transport capability based on the SP_3 approximation, a semi-analytical solution, and an advanced transverse leakage method based upon the use of analytic basis functions. Each of these new features is described followed by the results of benchmarks to test their effectiveness.

17/01804 An estimation to measure and to evaluate the work times following the trajectory of workers during decommissioning of nuclear facilities

Jeong, K. S. *et al. Annals of Nuclear Energy*, 2016, 94, 10–15.

This paper is intended to suggest an approach to an estimation of the work time to optimize the trajectories of workers during decommissioning of nuclear facilities. The working times during decommissioning for nuclear facilities have a great effect on safety and costs. The key feature of this work is to analyse and to evaluate the working times in virtual decommissioning environments. The measured data are statistically analysed into the mean and variance work time and radiation exposure dose. It is expected that the safety of decommissioning will be improved and decommissioning costs can be reduced. It can be concluded that this work will make it possible to efficiently establish the ALARA plan for decommissioning of nuclear facilities.

17/01805 Column experiment for assessing microbial behavior around radioactive waste repositories, including migration of potentially radionuclide-accumulating bacteria

Fukunaga, S. *et al. Applied Geochemistry*, 2016, 71, 99–109.

To assess microbial behaviour at anticipated repositories of nitrate-containing radioactive waste such as transuranic (TRU) waste, the authors set up an anoxic single horizontal column filled with Pleistocene sand with indigenous microorganisms as model samples. The column was supplied with artificial groundwater containing nitrate and acetate for 9 weeks (Run 1) or nitrate-amended groundwater from the same Pleistocene stratum for 6 weeks (Run 2). Bacterial communities, including culturable denitrifiers, were established in the sand bed, resulting in acridine orange direct counts per pore water of 3×10^8 cell mL^{-1} in Run 1 and 5×10^7 cell mL^{-1} in Run 2 and nitrate-reducing activity per pore water of roughly 13 mg L^{-1} d^{-1} in Run 1 and 1–4 mg L^{-1} d^{-1} in Run 2. Eh and hydraulic conductivity declined in Run 1, indicating microbial activity capable of retarding radionuclide transport. However, the ratio of bacterial cell concentration found in the effluent water (free-living bacteria) to the total bacterial concentration in sand (R_{mobile}) exceeded 2%. This finding is relevant to the increase in radionuclide transport associated with free-living cells. As a tool for quantifying this influence, the authors introduced an index, $K^{d,att}$ (distribution coefficient for microbes on sand particles), and calculated this value from the R_{mobile} value. By sensitivity analysis using a numerical simulation model (MINT), the authors then demonstrated that higher $K^{d,att}$ values would suppress the detrimental effects of the free-living bacteria. Quantification of microbial influences can be made more realistic by obtaining $K^{d,att}$ values in a column experiment and incorporating this index into radionuclide transport models.

17/01806 Economic competitiveness of small modular reactors versus coal and combined cycle plants

Alonso, G. *et al. Energy*, 2016, 116, 867–879.

Small modular reactors (SMRs) may be an option to cover the electricity needs of isolated regions, distributed generation grids and countries with small electrical grids. Previous analyses show that the overnight capital cost for SMRs is between 4500 and 5350 US$/kW, which is between a 6% and a 26% higher than the average cost of a current large nuclear reactor. This study analyses the economic competitiveness of small modular reactors against thermal plants using coal and natural gas combined cycle plants. To assess the economic competitiveness of SMRs, three overnight capital costs are considered 4500, 5000 and 5350 US$/kW along with three discount rates for each overnight cost considered, these are 3%, 7% and 10%. To compare with natural gas combined cycle (CC) units, four different gas prices are considered, these are 4.74 US$/GJ (5 US$/mmBTU), 9.48 US$/GJ (10 US$/mmBTU), 14.22 US$/GJ (15 US$/mmBTU) and 18.96 US$/GJ (20 US$/mmBTU). To compare against coal, two different coal prices are considered 80 and 120 US$/ton of coal. The carbon tax considered, for both CC and coal, is 30 US$/ton CO_2. The results show what scenarios make SMRs competitive against coal and/or combined cycle plants. In addition, because the price of electricity is a key component to guarantee the feasibility of a new project, this analysis calculates the price of electricity for the economically viable deployment of SMRs in all the above scenarios. In particular, this study shows that a minimum price of electricity of 175 US$/MWh is needed to guarantee the feasibility of a new SMR, if its overnight capital cost is 5350 US$/kWe and the discount rate is 10%. Another result is that when the price of electricity is around 100 US$/MWh then the discount rate must be around 7% or less to provide appropriate financial conditions to make SMRs economically feasible.

17/01807 Electricity generation mix and economic growth: what role is being played by nuclear sources and carbon dioxide emissions in France?

Marques, A. C. *et al. Energy Policy*, 2016, 92, 7–19.

The gradual trend towards the electrification of economies has raised new challenges. Focusing on France, this paper uses monthly data from January 2010 to November 2014, to study the challenge of the simultaneous integration of various sources of generation, and their relationship with economic growth. For the analysis of the dynamics of interaction between electricity sources, the auto-regressive distributed lag bounds test approach was shown to be appropriate, as it allows short- and long-run effects to be distinguished. The results showed that nuclear energy has been a huge driver of economic growth in France and, at the same time, leads to an environment with lower CO_2 emissions. Renewables were shown to exert a negative effect on economic growth, which could be due to lack of investment in other sources of production, due to the resilient position held by nuclear sources. The substitution effect among sources is noticeable. The robustness of the results was checked using annual data, from 1970 until 2012, and the results were comparable to those from the monthly data.

17/01808 Ensuring safety in design of safety critical computer based systems

Singh, L. K. and Rajput, H. *Annals of Nuclear Energy*, 2016, 92, 289–294.

Safety critical systems are designed to function in safe manner so that its failure should not lead to the catastrophic effects, including injury or death to humans, and harm to the environment. These systems take themselves to a safe state, thus ensuring goals of safety. Due to safety significance of such systems, these need to be designed carefully to ensure their reliability requirements. The strategy discussed the modelling and analysis techniques to safety critical computer based

systems using Petri net for full proof design. The techniques to improve the faulty design are also proposed. The application of the proposed techniques is shown on a reactor protection system.

17/01809 Evaluation of thermal hydraulic safety of a nuclear fuel assembly in a mast assembly of nuclear power plant

Kim, Y. S. *et al. Annals of Nuclear Energy*, 2016, 92, 136–149.

This study investigated the thermal–hydraulic safety of spent fuel bundles installed in a mast assembly, assuming a lock-up accident of a fuel transfer system. For this, flow analysis with computational fluid dynamics (CFD) for the natural convection and subsequent safety evaluation with 1-D nuclear power plant (NPP) safety analysis code were carried out. Prior to the natural convection analysis for the mast assembly using CFD code, the authors performed benchmark calculations against two experimental data sets obtained elsewhere. This was done to select the proper physical models for a natural convection flow analysis and to ensure the reliability of prediction of natural convection flow in the fuel bundle geometry. Finally, a main natural convection analysis was performed for the fuel assembly inside the mast assembly. From this calculation, the authors observed a stable natural circulation flow between the mast assembly and pool side, and obtained coolant velocity at the inlet of the spent fuel bundle. This flow condition is given as a boundary condition for the 1-D NPP safety analysis code, which is used to predict the critical heat flux and then departure from the nucleate boiling ratio.

17/01810 HAZOP application for the nuclear power plants decommissioning projects

Rimkevičius, S. *et al. Annals of Nuclear Energy*, 2016, 94, 461–471.

Decommissioning of nuclear facilities involves different types of activities, tools, equipment and systems. There is a potential for a wide range of radiological and industrial accidents during various stages of a decommissioning project creating risk for workers and the environment. The occurrence of accidents is possible due to many different operations involving movement and handling of large pieces of equipment and contaminated items. In addition, size reduction and decontamination processes are capable of producing hazards. One of the first steps in developing a safety assessment for decommissioning activities is the identification of hazards that can affect workers, members of the public and the environment during decommissioning activities, and then to identify engineered and administrative control measures to prevent, eliminate or mitigate the hazards and their consequences. Fault and hazard identification can be undertaken in several ways using a range of tools and techniques, including hazard and operability study (HAZOP). The paper will mainly focus on the application of HAZOP technique for identification of the hazards raised due to dismantling and decontamination activities at the Ignalina nuclear power plant, as well as at feasibility study for the management of Bohunice V1 nuclear power plant primary circuit components.

17/01811 Mechanical analysis of flying robot for nuclear safety and security control by radiological monitoring

Cho, H. S. and Woo, T. H. *Annals of Nuclear Energy*, 2016, 94, 138–143.

The flying robot is investigated for the nuclear accident and security treatment. Several mechanics are introduced for the movement of the drone. The optimized motion of the drone should cover all areas of nuclear power plants (NPPs) over the site where the circular and surmounting motions are needed with traverse of zigzag shapes. There is the yaw motion in the circular moving and the pitch motion in the climbing and downing against reactor facility. The fallout is calculated from the radiation concentration in the breaking part of the NPPs where the radioactive material leaks from the containment, coolant loop, plant facility and so on. The dose equivalents are obtained where the values are changeable following the random values of the y-value, average wind speed, and dispersed concentration in the detection position. The simulation of new positions of x, y and z are normalized from 0.0 to 1.0. The mechanics of flying robot produces the multidisciplinary converged technology incorporated with the aerial radiation monitoring information.

17/01812 The future of nuclear power in France: an analysis of the costs of phasing-out

Malischek, R. and Trüby, J. *Energy*, 2016, 116, 908–921.

Nuclear power is an important pillar in electricity generation in France. However, the French nuclear power plant fleet is ageing, and the possibility of reducing the technology's share in power generation or even a complete phase-out has been increasingly discussed. This paper focuses on three inter-related questions: first, what are the costs of phasing-out nuclear power in France? Second, who has to bear these costs, i.e. how much of the costs will be passed on to the rest of the European power system? And third, what effect does the uncertainty regarding future nuclear policy in France have on system costs? Applying a stochastic optimization model for the European electricity system, the analysis showed that additional system costs in France of a nuclear phase-out amount up to €76 billion (2010 value). Additional costs are mostly borne by the French power system. Surprisingly, the analysis found that the costs of uncertainty are rather limited. Based on the results, it can be concluded that a commitment regarding nuclear policy reform is only mildly beneficial in terms of system cost savings.

17/01813 Thinking big? Ghana, small reactors, and nuclear power

Ramana, M. V. and Agyapong, P. *Energy Research & Social Science*, 2016, 21, 101–113.

Ghana has been seen as a potential market for small nuclear reactors and Ghanaian nuclear officials have, on occasion, expressed an interest in such reactors. However, Ghana seems to be heading towards procuring a reactor from Russia with a capacity of 1000–1200 MW. A power plant with such a large power generation capacity is not appropriate to Ghana's limited electricity grid or its financial circumstances. This paper examines the likely reasons for this focus and argues that despite greater government interest in setting up nuclear reactors, Ghana's nuclear establishment may not have the political clout to force through the purchase of a reactor, and has therefore attempted to position itself as a complete, one-stop solution to Ghana's electricity crisis, by calling for the construction of just one or two large nuclear power plants. The paper draws on the role of discursive elements in energy policy making, discusses the policy implications of this reactor choice, and offers evidence for the proposition that decision about nuclear power are not made on the basis of merely techno-economic considerations but are driven by a range of social and political factors.

17/01814 Uncertainty analysis in post-accidental risk assessment models: an application to the Fukushima accident

Moustapha Sy, M. *et al. Annals of Nuclear Energy*, 2016, 93, 94–106.

Environmental contamination subsequent to the atmospheric releases during the Fukushima accident resulted in high radioactive concentrations in feed and foodstuffs. Producing a realistic health risk assessment after severe nuclear accidents, and developing a sufficient understanding of environmental transfer and exposure processes, appears to be a research priority. Specifically, the characterization of uncertainties in the human ingestion pathway, as outlined by the radioecological community, is of great interest. This work aims to (i) characterize spatial variability and parametric uncertainties raised by the processes involved in the transfer of radionuclides (^{134}Cs and ^{137}Cs) after atmospheric releases during the Fukushima accident into the terrestrial ecosystems, and (ii) study the impact of these variability and uncertainties on radioactive contamination of leafy vegetables. The implemented approach quantified uncertainties under a probabilistic modelling framework. This resulted in probability distributions derived mainly from Bayesian inference and by performing transfer calculations in the modelling platform SYMBIOSE.

17/01815 Updating of the public dose assessment approach for decommissioning related releases from the Ignalina NPP

Ragaišis, V. *et al. Annals of Nuclear Energy*, 2016, 94, 93–101.

The methodology used at the Ignalina nuclear power plant (NPP) for the assessment of the public exposure from radioactive releases to the environment is based on the use of so-called 'release-to-dose calculation factors' (RDFs). Application of RDFs is straightforward and in practice is used both to assess impacts from measured releases and to assess impacts from planned activities. The set of radionuclides and RDF values corresponding to them for operational releases were approved by the regulatory authorities. The decommissioning-related radiological characterization of the plant components and wastes revealed that the available set of RDFs is not sufficient for the decommissioning needs. To overcome this, a simplified approach has been proposed for the estimation of the missing RDF values. However, estimations using the simplified approach might be very inaccurate and not necessary conservative. This paper addresses the current practice of the dose assessment for releases from the Ignalina NPP and the necessity of extension of the available set of RDFs. New RDF values for the calculation of radiological impacts due to airborne releases from the power units and waterborne releases into Lake Drūkšiai are proposed for the decommissioning-relevant radionuclides. The significance of individual radionuclides in releases to the environment during decommissioning is discussed.

17/01816 Uranium demand and economic analysis of different nuclear fuel cycles in China

Zhang, J.-p. *et al. Energy Strategy Reviews*, 2016, 9, 50–61.

The demand of natural uranium of two different cycle options of China's pressurized water reactors (PWRs) were calculated in this paper, the once-through cycle route (OTC) is 197.2 t/8.702 TWh and

the partial recycling in PWR route (PRR) is 131.0 t/8.702 TWh. The fuel cycle component ($LCOE_{Total\ fuel\ cycle}$) of the levelized cost electricity (LCOE) for NPPS under different capacity, different cycle routes and different discount rate was calculated. In addition, the sensitivity analysis was made to identify the most influential parameters in the final price. Also, the breakeven price of uranium was calculated to be \$130/kg U for PRR fuel cycle with a fleet generating 100 TWh/year at 4% discount rate and \$74/kg U at 2% discount rate with reference to the OTC option. Then, the uncertainty analysis was made by Excel and Crystal software.

17/01817 Wishful thinking and real problems: small modular reactors, planning constraints, and nuclear power in Jordan

Ramana, M. V. and Ahmad, A. *Energy Policy*, 2016, 93, 236–245.

Jordan plans to import two conventional gigawatt scale nuclear reactors from Russia that are expensive and too large for Jordan's current electricity grid. Jordan efforts to establish nuclear power might become easier in some ways if the country were to construct small modular reactors, which might be better suited to Jordan's financial capabilities and its smaller electrical grid capacity. But, the small modular reactor (SMR) option raises new problems, including locating sites for multiple reactors, finding water to cool these reactors, and the higher cost of electricity generation. Jordan's decision has important implications for its energy planning as well as for the market for SMRs.

06 ELECTRICAL POWER SUPPLY AND UTILIZATION

Scientific, technical

17/01818 A linear programming model for power distribution with demand response and variable renewable energy

Babonneau, F. *et al. Applied Energy*, 2016, 181, 83–95.

A linear programming framework is proposed to model distribution network characteristics, and market clearing processes for flexible load and distributed energy resources providing reserve and reactive power compensation. One shows that the Nash equilibrium solution representing the interaction between utility and customers for demand response and distributed reserve transactions can be approximated by a linear program when the players (i.e. the customers) are numerous and tend to become infinitesimal. Then a linear programme is shown to reveal the market prices, corresponding to the marginal cost for the utility. The goal in developing this model is to provide a new module for a regional long term model of development of smart energy systems. This module will then introduce in the modelling of energy transition, the new options and constraints that are provided by a penetration of renewables with the possibility of implementing distributed markets for demand response and system services permitted by the development of the cyber-physical layer. A case study of a potential smart urban distribution network in Europe is carried out and provides numerical results that illustrate the proposed framework.

17/01819 A modified circuit topology for inductive pulsed power supply based on HTSPPTs

Li, H. *et al. Cryogenics*, 2016, 79, 38–44.

High temperature superconducting pulsed power transformer (HTSPPT) provides an efficient method for inductive energy storage and current multiplication. The primary inductor of HTSPPT used for energy storage is made of high temperature superconducting coils, and the secondary inductor used for current pulse generation is made of normal conductor coils. In the initial circuit, the secondary inductor generates current pulse by switching out the coupled primary superconducting inductor. However, during the switching period, the leakage flux caused by imperfect coupling and the sudden change in primary current induce a voltage across the opening switch which exceeds the affordability of modern solid-state switches. In previous studies, a half-cycle oscillatory discharge circuit is proposed to mitigate these problems by using a capacitor to recapture the energy in the leakage flux and to slow down the turnoff of current in the primary. However, there are still some problems should be settled. For example, the output pulse cannot be adjusted, the residual energy cannot be recovered and the capacitor branch circuit may have an impact on the charging process. In the paper, a modified discharge circuit topology is introduced to solve these problems. A multi-module system comprising of several HTSPPTs charging in series connection and discharging in parallel is also designed and simulated. This system can be used to power an electromagnetic emission device.

17/01820 A multi-objective optimization approach to optimal sensor location problem in IGCC power plants

Sen, P. *et al. Applied Energy*, 2016, 181, 527–539.

Integrated gasification combined cycle (IGCC) power plants provide a cleaner and more efficient way to obtain energy from coal. In order to operate an IGCC power plant in a safe and stable manner, several input and output process parameters need to be monitored. However, due to economic and operational constraints, it is infeasible to place sensors at every input and output process parameter location. Hence, it becomes important to select the most effective sensor locations which lead to maximum information gain about the plant conditions. Practical issues present in an IGCC power plant, such as harsh physical conditions and variability in process parameters, make the optimal sensor location problem an especially complicated one. Further, sensors can have multiple objectives and they can produce uncertainties due to measurement errors. This work considers hybrid hardware and virtual sensing for advanced power systems with multiple objectives. In order to solve this real world large-scale problem, a novel algorithm was used called 'Better Optimization of Non-linear Uncertain Systems' (BONUS). BONUS works in probability distribution space and avoids sampling for each optimization and derivative calculations iterations. A new algorithm for multi-objective optimization is also developed specifically for problem. The result of this non-linear stochastic multi-objective problem is the non-dominated, or Pareto set, which provides trade-offs between various objectives like observability, cost, and thermal efficiency. This is the first attempt at solving the problem of optimal sensor deployment in advanced power plants, with consideration of hybrid hardware and virtual sensing and incorporation of uncertainty with multiple objectives.

17/01821 Corrective economic dispatch and operational cycles for probabilistic unit commitment with demand response and high wind power

Azizipanah-Abarghooee, R. *et al. Applied Energy*, 2016, 182, 634–651.

In this study, the authors propose a probabilistic unit commitment problem with incentive-based demand response and high level of wind power. A novel formulation provides an optimal allocation of up/down spinning reserve. A more efficient unit commitment algorithm based on operational cycles is developed. A multi-period elastic residual demand economic model based on the self- and cross-price elasticities and customers' benefit function is used. In the proposed scheme, the probability of residual demand falling within the up/down spinning reserve imposed by $n-1$ security criterion is considered as a stochastic constraint. A chance-constrained method, with a new iterative economic dispatch correction, wind power curtailment, and commitment of cheaper units, is applied to guarantee that the probability of loss of load is lower than a pre-defined risk level. The developed architecture builds upon an improved Jaya algorithm to generate feasible, robust and optimal solutions corresponding to the operational cost. The proposed framework is applied to a small test system with 10 units and also to the IEEE 118-bus system to illustrate its advantages in efficient scheduling of generation in the power systems.

17/01822 Decentralized voltage control of clustered active distribution network by means of energy storage systems

Bahramipanah, M. *et al. Electric Power Systems Research*, 2016, 136, 370–382.

The paper presents a network partitioning strategy for the optimal voltage control of active distribution networks (ADNs) actuated by means of a limited number of distributed energy storage systems (DESSs). The proposed partitioning uses a linear programming approach by means of the known concept of voltage sensitivities. Then, two decentralized optimal control algorithms are proposed relying, respectively, on the Thévenin equivalents and a recursive approach. These algorithms are developed using the multi-agent system concept. With respect to a centralized control algorithm, the aim of the network clustering is to reduce the number of exchanged messages among the clusters when one of the two proposed decentralized control algorithms is adopted. The effectiveness of the two proposed controls is assessed with respect to the performances of the equivalent centralized control using numerical examples composed by the IEEE 13 and IEEE 123 buses distribution test feeders adapted to include stochastic generation and DESSs.

17/01823 Design and thermodynamic analysis of a flash power system driven by process heat of continuous casting grade steel billet

Sun, W. and Zhang, F. *Energy*, 2016, 116, 94–101.

Hot charging of continuous cast steel billets is usually considered an effective method for recovering heat. However, for certain grades of steel, the hot charging process may affect the steel surface quality. To overcome this issue, the billet is commonly cooled down before rolling, resulting in substantial heat loss. Thus, the recovery of useful waste heat without affecting steel quality is an important research topic. In this study, the design of a flash power system driven by the process heat of continuous casting grade steel billet is proposed. The influences of shunted water temperature and flash pressure on exergy recovery rate are studied via the thermodynamic methods. Moreover, a case study based on actual data is analysed to verify the thermodynamic results and the energy recovery of the proposed system. The results indicate that the system exergy recovery rate increases with increasing shunted water temperature. Keeping the shunted temperature unchanged the exergy recovery rate firstly increases and later decreases with increasing flash pressure. At a fixed shunt temperature, an optimum flash pressure exists. At the maximum exergy recovery rate the net output power of the studied plant is 6361 kW, a value that greatly reduces the need for purchased electricity.

17/01824 Target-oriented robust optimization of polygeneration systems under uncertainty

Sy, C. L. *et al. Energy*, 2016, 116, 1334–1347.

Production of clean, low-carbon energy and by-products is possible through the use of highly integrated, efficient systems such as polygeneration plants. Mathematical programming methods have proven to be valuable for the optimal synthesis of such systems. However, in practice, numerical parameters used in optimization models may be subject to uncertainties. Examples include cost coefficients in volatile markets, and thermodynamic coefficients in new process technologies. In such cases, it is necessary for the uncertainties to be incorporated into the optimization procedure. This paper presents a target-oriented robust optimization (TORO) approach for the synthesis of polygeneration systems. The use of this methodology leads to the development of a mathematical model that maximizes robustness against uncertainty, subject to the achievement of system targets. Its properties allow us to preserve computational tractability and obtain solutions to realistic-sized problems. The methodology is demonstrated for the synthesis of polygeneration systems using TORO with an illustrative case study.

17/01825 Temporal and spatial tradeoffs in power system modeling with assumptions about storage: an application of the POWER model

Frew, B. A. and Jacobson, M. Z. *Energy*, 2016, 117, 198–213.

As the number and complexity of power system planning models grows, understanding the impact of modelling choices on accuracy and computational requirements becomes increasingly important. This study examines empirically various temporal and spatial trade-offs using the POWER planning model for scenarios of a highly renewable US system. First, the common temporal simplification of using a representative subset of hours from a full year of available hours is justified using a reduced form model. Accuracy losses are generally $\leq$6%, but storage is sensitive to the associated model modifications, highlighting the need for proper storage balancing constraints. Cost trade-offs of various temporal and spatial adjustments are then quantified: four temporal resolutions (1- to 8-h-average time blocks); various representative day subset sizes (1 week to 6 months); two spatial resolutions of site-by-site versus uniform fractional buildout across all solar and wind sites; and multiple spatial extents, ranging from California to the contiguous USA. Most trade-offs yield <15% cost differences, with the effect of geographic aggregation across increasing spatial extents producing the largest cost reduction of 14% and 42% for the western and contiguous USA, respectively. These results can help power system modellers determine the most appropriate temporal and spatial treatment for their application.

17/01826 The effects of the voltage recovery after the voltage sag on gas discharge lamps

Sengul, M. *Electric Power Systems Research*, 2016, 136, 309–321.

Power quality has become a major focal point for many utilities. One of the most common power quality issues that consumers deal with is the voltage sag. This study leads to understanding of electrical behaviour of different types of gas discharge lamps after the recovery of the voltage at the end of a sag. The analysed discharge lamps are fluorescent lamps, low- and high-pressure sodium lamps, metal halide lamps and tungsten halide lamps. Extensive laboratory tests were carried out for detecting the effects of the voltage sag duration and magnitude on these lamps. From the analysis of the test findings, it was seen that some conditions cause a current spike (inrush current) on gas discharge lamps upon voltage recovery. It was concluded that the magnitude of the current spike on the lamps depends on not only the magnitude of the sag, but also the duration of the voltage sag.

17/01827 Thermodynamic analysis of parabolic trough and heliostat field solar collectors integrated with a Rankine cycle for cogeneration of electricity and heat

Shahin, M. S. *et al. Solar Energy*, 2016, 136, 183–196.

Nowadays the production of electricity still relies heavily on the use of fossil fuels and is a main factor in environmental pollution. Therefore, clean alternative sources are needed for the production of electricity. In recent years, the use of renewable energy has become more prevalent in everyday lives due to an increased environmental awareness worldwide. Solar energy emanating from the sun is used in agriculture, thermal heating, and electricity production. This study proposes a model that integrates a solar harvesting system of collectors that heat up a heat transfer fluid into a conventional Rankine cycle for the production of electricity and thermal power. In this regard, a thermodynamic analysis of the proposed model is performed to evaluate and improve its performance. The analysis consists of an assessment of energy equations extracted from literature and theory books for each subsystem; the solar collectors (a parabolic trough and a heliostat field); and the Rankine cycle. These equations are used to simulate the performance of the overall system under constant solar irradiation. Moreover, a parametric study is carried out to determine the effect of various design and operation parameters on the overall efficiency and power output. Furthermore, a comparative analysis of the parabolic trough and the heliostat field is presented in order to determine the optimum option to couple with the proposed model. The different operating conditions include several solar irradiation intensities, geometric values of the collectors, mass flow rates of the heat transfer fluids, and temperature values. The results show that the heliostat field achieves a better performance in comparison to the parabolic trough.

17/01828 Thermoelectric power waves from stored chemical energy

Singh, S. *et al. Energy Storage Materials*, 2016, 3, 55–65.

Thermopower wave is a new concept of energy conversion where the chemical energy stored in solid fuel is directly converted into electricity. In this review article, the concept and recent progress of thermopower wave investigations were discussed. The self-sustained reaction propagation of fuels coated around thermal conduit was first theoretically suggested and experimentally realized using a shell–core structure of cyclotrimethylene-trinitramine coated multi-walled carbon nanotubes. The exothermic chemical reaction of fuel was guided and accelerated by the thermal conduit with greater thermal conductivity. The temperature gradient at the reaction front also resulted in electrical pulse caused by the Seebeck effect. However, the peak output voltage was limited to $\sim$210 mV due to the low Seebeck coefficient of carbon nanotubes. In order to further enhance the peak output voltage after the first discovery, research efforts have been focused on three areas; thermal conduit with greater Seebeck coefficients, geometric structures of fuel/conduits, and different types of chemical fuels. The thermal conduits with greater Seebeck coefficients generally provided higher peak voltages. One-dimensional structure of fuel/conduits generated more efficient thermopower waves than two- or three-dimensional structures. Picric acid with self-aligned one-dimensional structure could also accelerate the reaction propagation. Overall, the peak output voltage was enhanced from $\sim$210 mV to 6.2 V in only 5 years of research demonstrating the rapid advance and bright future of thermopower waves.

17/01829 Thermostable gel polymer electrolyte based on succinonitrile and ionic liquid for high-performance solid-state supercapacitors

Pandey, G. P. *et al. Journal of Power Sources*, 2016, 328, 510–519.

A flexible, free-standing, thermostable gel polymer electrolyte based on plastic crystalline succinonitrile (SN) and ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate ($BMImBF_4$) entrapped in copolymer poly(vinylidene fluoride-*co*-hexafluoropropylene) (PVdF-HFP) is prepared and optimized for application in solvent-free solid-state supercapacitors. The synthesized gel polymer electrolyte exhibits a high ionic conductivity over a wide temperature range (from $\sim 5 \times 10^{-4}$ S cm^{-1} at -30 °C up to $\sim 1.5 \times 10^{-2}$ S cm^{-1} at 80 °C) with good electrochemical stability window (-2.9 to 2.5 V). Thermal studies confirm that the SN containing gel polymer electrolyte remains stable in the same gel phase over a wide temperature range from -30 to 90 °C. The electric double layer capacitors (EDLCs) have been fabricated using activated carbon as active materials and new gel polymer electrolytes. Electrochemical performance of the EDLCs is assessed through cyclic voltammetry, galvanostatic charge-discharge cycling and impedance spectroscopy. The EDLC cells with the proper SN-containing gel polymer electrolyte has been found to give high specific capacitance 176 F g^{-1} at 0.18 A g^{-1} and 138 F g^{-1} at 8 A g^{-1}. These solid-state EDLC cells show good cycling stability and the capability to retain $\sim$80% of the initial capacitance after 10,000 cycles.

17/01830 Vanadium based materials as electrode materials for high performance supercapacitors
Yan, Y. *et al. Journal of Power Sources*, 2016, 329, 148–169.
As a kind of supercapacitors, pseudocapacitors have attracted wide attention in recent years. The capacitance of the electrochemical capacitors based on pseudocapacitance arises mainly from redox reactions between electrolytes and active materials. These materials usually have several oxidation states for oxidation and reduction. Many research teams have focused on the development of an alternative material for electrochemical capacitors. Many transition metal oxides have been shown to be suitable as electrode materials of electrochemical capacitors. Among them, vanadium based materials are being developed for this purpose. Vanadium based materials are known as one of the best active materials for high power/energy density electrochemical capacitors due to its outstanding specific capacitance and long cycle life, high conductivity and good electrochemical reversibility. There are different kinds of synthetic methods such as sol-gel hydrothermal/solvothermal method, template method, electrospinning method, atomic layer deposition, and electrodeposition method that have been successfully applied to prepare vanadium based electrode materials. This review provides an overall summary and evaluation of the recent progress in the research of vanadium based materials for electrochemical capacitors that include synthesis methods, the electrochemical performances of the electrode materials and the devices.

Economics, policy, supplies, forecasts

17/01831 A bibliometric analysis based review on wind power price
Gao, C. *et al. Applied Energy*, 2016, 182, 602–612.
With the increasing negative effects of fossil fuel combustion, many countries have paid more attention on supporting environmentally friendly energy generation, particularly renewable and sustainable energy sources. However, renewables still cannot economically compete with fossil-fuels and are facing new challenges. Appropriate electricity pricing mechanism plays a vital role on mitigating the stress of limited fossil fuels and can promote renewable energy consumption. As one major type of renewable energy, wind power has been globally promoted. In order to promote the application of wind power, appropriate wind power prices should be established by considering the local conditions. This paper targets such a field and conducts a bibliometric and network analysis based on the data from Scopus. The results show that the numbers of total related publications are gradually increasing, with the USA as the leading country. European countries also have outstanding achievements. Moreover, both the most cited articles and keywords distribution offer future research directions. In general, this study provides valuable insights to both wind power researchers and practitioners.

17/01832 A field study of human factors and vehicle performance associated with PHEV adaptation
Farhar, B. C. *et al. Energy Policy*, 2016, 93, 265–277.
Smart-grid and electric-vehicle technologies are rapidly diffusing, yet important policy implications remain to be fully analysed. This multi-year field study sought to fill part of this gap by exploring human adaptation to plug-in hybrid electric vehicle (PHEV) performance and vehicle charging in smart-grid environments. Homes were equipped with smart meters in a smart-grid experiment conducted by the local utility. Study households were organized by either standard or time-of-use electricity pricing, and randomly assigned to 'managed' or 'unmanaged' charging scenarios. Using a mixed-methods approach, study data were collected through vehicle data loggers, smart-plugs interviews, and questionnaires. The paper describes vehicle operations and performance; the ways in which households managed PHEV charging; and the manner in which they responded to smart-grid, smart-plug, and dashboard feedback. Findings indicate that households actively managed PHEV charging; however, they preferred flexible charging scenarios. Charging-management decisions were influenced by electricity-pricing. Online feedback on household- and vehicle-electricity consumption was generally ignored, but drivers responded to dashboard feedback as they drove. These results provide empirical bases for government and corporate policymakers to improve policy decisions relative to PHEV impacts on electricity loads, design of smart-grid feedback, and design of charging infrastructures.

17/01833 A novel centralized charging station planning strategy considering urban power network structure strength
Pan, Z.-j. and Zhang, Y. *Electric Power Systems Research*, 2016, 136, 100–109.
Considering detrimental impact on grid by sizeable and unpredictable electric vehicles (EVs) loads, establishing centralized charging stations through swapping batteries can be the future competitive development orientations in EV industry. Optimal centralized charging station planning is not only pervasive enough to meet the requirement of EV charging, but also has the potential to improve the rationality of power grid structure as a distributed power station. In this paper, a novel centralized charging station strategy considering urban power network structure strength is proposed. Based on the analysis of time-space characteristic of load shifting in normal urban life, power supply moment balance index is defined to represent fluctuation of supply capability between peak and valley under certain structure. Meanwhile, the investment of charging stations and network loss are considered as part of objective function with moment balance index, aiming at improving urban power network structure with minimal economic cost. Case study on IEEE 123-bus test distribution system illustrates the validity of the strategy proposed.

17/01834 A profitability assessment of small-scale photovoltaic systems in an electricity market without subsidies
Cucchiella, F. *et al. Energy Conversion and Management*, 2016, 129, 62–74.
The installation of photovoltaic power plants in 2015 compared to 2014 registered a growth of 25.6%, reaching a cumulative power equal to 229 GW. In developed solar markets, as many European countries, the sector is pushed by the alignment between the electric power demanded and the one offered. Consequently, self-consumption makes consumers active players of the energy transition. Italy is evaluated as a case study in this paper, in fact is the first country in the world where solar energy contributes largely to the national energetic demand. This paper aims to evaluate photovoltaic systems in residential sector without subsidies. Economic and environmental results are proposed and the indicators used are net present value, discounted payback time and reduction in the emissions of carbon dioxide. Three sizes (3, 6 and 20 kW) are evaluated. In addition, a sensitivity analysis of critical variables (investment cost, annual electricity purchase price, annual electricity sales price, opportunity cost, tax deduction unitary, period of fiscal deduction, average annual insolation and percentage of energy self-consumption) demonstrates the robustness of the economic results. Also for environmental evaluation, alternative scenarios are proposed varying the value of emissions released by source energy analysed (photovoltaic, coal, oil and gas). Economic and environmental results suggest that small-scale photovoltaic systems can support the transition towards a sustainable energy mix.

17/01835 A systematic design of interval type-2 fuzzy logic system using extreme learning machine for electricity load demand forecasting
Hassan, S. *et al. International Journal of Electrical Power & Energy Systems*, 2016, 82, 1–10.
This paper presents a novel design of interval type-2 fuzzy logic systems (IT2FLS) by utilizing the theory of extreme learning machine (ELM) for electricity load demand forecasting. ELM has become a popular learning algorithm for single hidden layer feed-forward neural networks (SLFN). From the functional equivalence between the SLFN and fuzzy inference system, a hybrid of fuzzy-ELM has gained attention of the researchers. This paper extends the concept of fuzzy-ELM to an IT2FLS based on ELM (IT2FELM). In the proposed design the antecedent membership function parameters of the IT2FLS are generated randomly, whereas the consequent part parameters are determined analytically by the Moore–Penrose pseudo inverse. The ELM strategy ensures fast learning of the IT2FLS as well as optimality of the parameters. Effectiveness of the proposed design of IT2FLS is demonstrated with the application of forecasting non-linear and chaotic data sets. Nonlinear data of electricity load from the Australian National Electricity Market for the Victoria region and from the Ontario Electricity Market are considered here. The proposed model is also applied to forecast Mackey-glass chaotic time series data. Comparative analysis of the proposed model is conducted with some traditional models such as neural networks (NN) and adaptive neuro fuzzy inference system (ANFIS). In order to verify the structure of the proposed design of IT2FLS an alternate design of IT2FLS based on Kalman filter (KF) is also utilized for the comparison purposes.

17/01836 An examination of electricity generation by utility organizations in the southeast United States
Craig, C. A. and Feng, S. *Energy*, 2016, 116, 601–608.
This study examined the impact of climatic variability on electricity generation in the south-east USA. The relationship cooling degree days (CDDs) and heating degree days (HDDs) shared with electricity generation by fuel source was explored. Using seasonal autoregressive integrated weighted average (ARIMA) and seasonal simple exponentially smoothed models, retrospective time series analysis was run. The hypothesized relationship between climatic variability and total elec-

tricity generation was supported, where an ARIMA model including CDDs as a predictor explained 57.6% of the variability. The hypothesis that climatic variability would be more predictive of fossil fuel electricity generation than electricity produced by clean energy sources was partially supported. The ARIMA model for natural gas indicated that CDDs were the only predictor for the fossil fuel source, and that 79.4% of the variability was explained. Climatic variability was not predictive of electricity generation from coal or petroleum, where simple seasonal exponentially smoothed models emerged. However, HDDs were a positive predictor of hydroelectric electricity production, where 48.9% of the variability in the clean energy source was explained by an ARIMA model. Implications related to base load electricity from fossil fuels, and future electricity generation projections relative to extremes and climate change are discussed.

17/01837 An intelligent θ-modified bat algorithm to solve the non-convex economic dispatch problem considering practical constraints

Kavousi-Fard, A. and Khosravi, A. *International Journal of Electrical Power & Energy Systems*, 2016, 82, 189–196.

This paper proposes a practical formulation for the non-convex economic dispatch problem to consider multi-fuel options, ramp rate limits, valve loading effect, prohibited operating zones and spinning reserve. A new optimization algorithm based on the θ-bat algorithm (θ-BA) is suggested to solve the problem. The θ-BA converts the Cartesian search space into the polar coordinates such that more search ability would be achieved. According to the complex, non-linear, and constrained nature of the problem, a new self-adaptive modification method is proposed. The proposed modified θ-BA (θ-MBA) is constructed based on the roulette wheel mechanism to effectively increase the convergence of the algorithm. The high ability and satisfying performance of the proposed optimization method is examined on IEEE 15-unit, 40-unit and 100-unit test systems.

17/01838 Assessment of the macroeconomic and sectoral effects of higher electricity and gas prices in the EU: a general equilibrium modeling approach

Capros, P. *et al. Energy Strategy Reviews*, 2016, 9, 18–27.

The macroeconomic and sectoral effects of differentials in energy prices between the EU and the non-EU countries in the horizon to 2050 are assessed with the use of GEM-E3, a computable general equilibrium model. Alternative scenario variants are quantified: In the first case, EU policies and market structures regarding taxation, penetration of renewable energy sources in power generation and higher market power of EU energy producers lead to higher EU energy prices compared to those recorded in the non-EU countries. In the second variant developments in non-EU countries lead to lower energy prices as compared to those in the EU. Simulation results show that higher EU energy prices lower EU gross domestic product compared to the baseline case. The impact ranges in magnitude between 0.02% and 0.41%, cumulatively over 2015–2050, depending on the drivers of price differentials and on the use of the additional tax revenues generated. Taxation and power generation mix policies are found to have the largest impact on economic activity. The results indicate the challenges of electricity and gas price developments that EU policy making needs to address in the following years so as to ensure long-term competitiveness and growth.

17/01839 Beyond decide-announce-defend (DAD) and not-in-my-backyard (NIMBY) models? Addressing the social and public acceptance of electric transmission lines in Germany

Komendantova, N. and Battaglini, A. *Energy Research & Social Science*, 2016, 22, 224–231.

Energy transition in Germany requires deployment of new electricity transmission infrastructure, such as new electricity grids, which faces opposition of communities, where infrastructure is planned. Scientific evidence on differences in social and public acceptance is limited and in combination to a particular type of infrastructure, such as electricity transmission networks, is almost non-existent. Also there is an additional need to understand how acceptance, which is more a passive attitude towards something imposed top-down, can be changed to willingness of participation. Based on several methods of stakeholders dialogue such as survey, feedback forms and observation on the site of public information events, this paper addresses social and public acceptance issues in two electricity transmission pilot projects. In doing so, it advances, tests, and refines core tenets from two major streams of thought related to NIMBY (not-in-my-backyard) and decide–announce–defend (DAD) concepts. The study analyses these themes through a comparison of the Sued.Link connection being realized by the transmission system operator TenneT and the Bertikow–Pasewalk connection being realized by 50Hertz. The results allow us to identify major concerns regarding these two pilot projects as well as to provide recommendations on successfulness of the actions to address these concerns.

17/01840 Bribes, bureaucracies, and blackouts: towards understanding how corruption at the firm level impacts electricity reliability

Pless, J. and Fell, H. *Resource and Energy Economics*, 2017, 47, 36–55.

This paper looks at whether bribes for electricity connections affect electricity reliability. Using detailed firm-level data, the authors estimate various specifications based upon repeated cross-sections and means-based pseudo-panels to show that bribes are closely related to poorer electricity reliability. It was found that the propensity to bribe for an electricity connection is associated with an increase of 14 power outages per month and a 22% increase in annual sales lost due to power outages on average. The results parallel a tragedy of the commons story: electricity, which exhibits common-pool resource characteristics, suffers from overexploitation as self-interested individual firms rationally bribe for electricity, creating negative impacts in aggregate on the overall quality of the resource. Given the importance of electricity reliability for economic growth and development, the findings imply that improving oversight and enforcement measures at the consumer level that target the reduction of bribery for electricity connections could contribute to growth and development.

17/01841 On representation of temporal variability in electricity capacity planning models

Merrick, J. H. *Energy Economics*, 2016, 59, 261–274.

This paper systematically investigates how to represent intra-annual temporal variability in models of optimum electricity capacity investment. Inappropriate aggregation of temporal resolution can introduce substantial error into model outputs and associated economic insight. The mechanisms underlying the introduction of this error are shown. How many representative periods are needed to fully capture the variability is then investigated. For a sample dataset, a scenario-robust aggregation of hourly (8760) resolution is possible in the order of 10 representative hours when electricity demand is the only source of variability. The inclusion of wind and solar supply variability increases the resolution of the robust aggregation to the order of 1000. A similar scale of expansion is shown for representative days and weeks. These concepts can be applied to any such temporal dataset, providing, at the least, a benchmark that any other aggregation method can aim to emulate. How prior information about peak pricing hours can potentially reduce resolution further is also discussed.

17/01842 Opening the black box of energy security: a study of conceptions of electricity security in the United Kingdom

Cox, E. *Energy Research & Social Science*, 2016, 21, 1–11.

Despite much literature on energy security, the term continues to resist a commonly-accepted definition. Nevertheless, policy decisions are frequently made on the basis of 'improving energy security', despite the lack of any clear understanding of what improving energy security actually means. Therefore this paper explores the meaning of energy security for key experts in the UK energy sector, with a particular focus on the security of electricity systems in the context of a low-carbon transition. A set of 22 energy security issues is discussed with 25 experts from across the energy sector in the UK, in order to get a grasp on which aspects of energy security are felt to be most important, and to discover the underlying concepts which are used by experts when making or justifying these choices. The results from the interviews show that there is a real need to attempt to take into account multiple competing and context-specific views on energy security, instead of trying to close the discussion down around a small number of simple quantifiable indicators or metrics. The results also show that there is no clearly discernible alignment between experts' perspectives and the type of organization for which they work.

17/01843 Optimal design of distributed energy system in a neighborhood under uncertainty

Akbari, K. *et al. Energy*, 2016, 116, 567–582.

Distributed energy systems (DES) are widely accepted as the future generation of the energy systems. The number of studies in all related fields corroborates the assertion that these systems are in their infancy and need to develop more in terms of efficiency and economizing. Admittedly, these systems are hardly lucrative and poor planning is one of many hurdles standing in the way of their profitability. Disregarding uncertainty as an innate characteristic of the real world seems one of the improper simplifications of this planning. To cover this gap, the paper is mainly focused on designing an energy system in a neighbourhood including its pipeline network under demand uncertainty concerning data insufficiency. Therefore, a new model for planning in a neighbourhood is presented and then reformulated to its robust counterpart. Various technologies like photovoltaic arrays, chillers, boiler, storage tank, and combined heat and power plants are considered in order to meet the cooling, heating and electrical demands. The probable consequences of the demand uncertainty are studied to the length. The outcomes reveal that the unit sizes and pipeline network are highly dependent on the decision maker's level of conservatism.

17/01844 Optimal scheduling of dispatchable distributed generation in smart environment with the aim of energy loss minimization
Rahiminejad, A. *et al. Energy*, 2016, 116, 190–201.
It is obvious that the high accurate information of network conditions in smart grids definitely leads to high efficient performance of the network. This paper discusses how much is the effect of smart grid compared to conventional networks to the daily energy loss minimization. In other words, the question of 'is it worth to move towards the smart environment?' is discussed from only an aspect point of view in the paper. For this purpose, an optimal management of dispatchable distributed generation (DDG) in smart grid with the aim of daily energy loss minimization is performed and fairly compared to DDG optimal management in conventional distribution networks. The effect of suboptimal performance of the system in conventional networks is economically analysed. A three-level load profile which is forecasted in advance is taken into account as the load profile of the conventional network. This load profile is investigated in five different scenarios from prediction points of view. On contrary, the load profile of the network in smart environment is considered as a 24-h load profile which is achieved using smart metering devices. To show how the smart grid impressively affects the network performance regards to conventional network, the DDGs are also programed in order to minimize the voltage deviation of the network. The economic analysis and yearly benefit of loss reduction are also conducted in both situations (smart grid and conventional network). In addition, the performances of the conventional network and smart grid are evaluated in two other phases, i.e. in the presence of renewable energy resources and encountering with disturbances. The study is applied on 69-bus radial test system which is used in many previous studies. The results show the detrimental effects of suboptimal operation of the system on network performance in the case of conventional networks. Moreover, the impressive impacts of smart environment on energy loss reduction and voltage profile improvement in distribution systems can be concluded from the results. Furthermore, the study shows how the smart environment can be useful for utilization of renewable energy resources and managing the disturbances.

17/01845 Winds of change in energy systems: policy implementation, technology deployment, and regional transmission organizations
Stafford, B. A. and Wilson, E. J. *Energy Research & Social Science*, 2016, 21, 222–236.
Changes in the electricity sector since the turn of the century have brought significant penetration of wind generation resources onto the electric power grid. Creating a low-carbon and sustainable electric systems to respond to climate change and meet societal energy needs requires different technologies and changes in supporting policies and institutions. But just how these institutions are creating and implementing new policies has emerged as an important area of inquiry. Changing how the electricity system works requires coordinated interaction across many different stakeholder groups and multiple levels of governance. The authors explore these emerging processes of policy implementation by examining how wind energy resources are changing the operation of the electric grid. To do this, an in-depth, grounded case study examining decision making within the Midcontinent Independent System Operator (MISO), a US regional transmission organization was developed. A multi-method approach was applied to the strategic action field theory to examine how MISO created and implemented policy, changing energy markets and power systems operation to allow for the integration of wind resources. This study examines the critical and understudied role of energy policy implementation in practice and focuses on how stakeholders are making decisions which are shaping the use and value of new and existing energy technologies and, in doing so, transforming the energy system.

07 STEAM RAISING

Boiler operation/design

17/01846 A review of some operation and maintenance issues of CFBC boilers
Arjunwadkar, A. *et al. Applied Thermal Engineering*, 2016, 102, 672–694.
Circulating fluidized bed (CFB) technology has emerged as the most favoured steam generation technology in recent times. The use of CFB boilers is growing exponentially, due to its attractive features such as fuel flexibility, stable operation and low acid gas emissions, to name a few. The design of CFB boilers has developed over the years to meet the demanding availability expectations of the utilities. Proactive operation and maintenance (O&M) helps improve availability and reduce operating costs, which form a crucial component of the final steam cost of the boiler plant. This paper studies some important O&M issues of CFB boilers particularly looking into issues related to components specific to CFB boilers and the methods to avoid them. Operational difficulties like agglomeration, gas refluxing, back-sifting and performance related issues like emission control and bed temperature control are also examined. Refractory failure, which accounts for a considerable portion of the maintenance cost often forces shutdowns. This review is based on compilation of O&M issues of CFB boiler as found mainly in the open literature, but some unpublished information are also included.

17/01847 Effect of different inner secondary-air vane angles on combustion characteristics of primary combustion zone for a down-fired 300-MW_e utility boiler with overfire air
Wang, Q. *et al. Applied Energy*, 2016, 182, 29–38.
To achieve significant reductions in NO_x emissions without increasing the levels of unburnt carbon in the fly ash, a new combustion system was applied to a 300-MW_e Babcock and Wilcox down-fired boiler installed with swirl burners. The unit featured introduced overfire air and decreased outlet area of the inner and outer secondary-air ducts of the swirl burners. Full-scale measurements (adjusting the inner secondary-air vane angle to 35°, 45° and 55°) revealed that the influence of the high-temperature recirculating region under the arch upon the combustion and NO_x emission characteristics of the boiler is greater than that of the high-temperature flue gas entrained by the swirl burner itself. The ignition distance of the coal/air flow is reduced by at least 1.8 m compared with that of the original combustion system. For the inner secondary-air vane angle of 35°, the coal/air flow ignites earlier than for the vane angles of 45° and 55°. The measurements of the gas species concentrations in the zone near the sidewall indicates that at inspection port 1, the coal flame of the burners does not spread across the entire furnace cross-section for all three vane angles; however, for the vane angle of 35° the flame is spread across the entire furnace cross-section at inspection port 2. For this optimal (35°) inner secondary-air vane angle, the NO_x emissions and carbon content in the fly ash reached levels of 674 mg/m^3 (6% O_2), and 11.4%, respectively, achieving a significant NO_x reduction of 51.9% without increasing the levels of unburnt carbon in the fly ash.

17/01848 Effective boundary conditions and turbulence modeling for the analysis of steam turbine exhaust hood
Veerabathraswamy, K. and Kumar, A. S. *Applied Thermal Engineering*, 2016, 103, 773–780.
The steam turbine exhaust hood is a stationary component which connects the last stage of the turbine exit to the condenser. An optimal geometric design of the exhaust hood is typically achieved through multiple design iterations in conjunction with computational methods estimating the performance of every such design. To satisfy the need of quick performance estimation, a reduced computational model with the inlet of the computational domain at the trailing edge plane of the last stage rotor is commonly used. The main challenge in using a reduced computational model is selection of appropriate inlet and outlet boundary conditions, as the flow condition at these boundaries are not known. In this work, the boundary condition options for the outlet where a significant reverse flow is expected are studied, along with studying the effect of condenser tubes on the flow regime. Use of total pressure, mass flow rate and velocity boundary conditions at the inlet along with extended domain options are evaluated for inlet boundary modelling. In addition, a comprehensive study of turbulence models with respect to their ability to predict the pressure loss is reported. A recommendation on the turbulence model and boundary conditions for the exhaust hood modelling is arrived at, which is validated with experimental results. The implementation of recommended inlet, outlet boundary conditions and turbulence model produced consistent results with 9% reduced computational effort.

17/01849 Estimation of exhaust steam enthalpy and steam wetness fraction for steam turbines based on data reconciliation with characteristic constraints
Guo, S. *et al. Computers & Chemical Engineering*, 2016, 93, 25–35.
Wetness fraction of exhaust steam is important to the economy and safety of steam turbines. Due to lack of commercially available measurement technologies, it is usually obtained from model based calculation via other measurements. However, accuracy of relevant measurement data is usually unsatisfactory due to limits of measuring instruments, and data reconciliation can be applied to improve the

accuracy of these measurements. Traditionally, balance constraints of steam turbines are mostly considered in data reconciliation, and results of previous studies illustrate that there is still potential for further improvement. This work presents a generalized data reconciliation approach with both balance and characteristic constraints for estimation of wet steam parameters in steam turbines, with case studies on a real-life 1000 MW coal-fired power plant. The results show that uncertainty reduction is enhanced for all measurements. Better estimates of exhaust steam enthalpy and steam wetness fraction can be therefore obtained after data reconciliation.

17/01850 Experimental study of a parabolic trough solar collector with flat bar-and-plate absorber during direct steam generation

Bortolato, M. *et al. Energy*, 2016, 116, 1039–1050.

The present work aims at investigating an innovative flat aluminium absorber for process heat and direct steam generation in small linear solar concentrating collectors. After defining its optimal width through a Monte Carlo ray-tracing analysis, this absorber has been manufactured with the bar-and-plate technology, including an internal offset strip turbulator in the channel. This technology is cost-effective and extremely flexible, allowing to easily adapt the geometry of the absorber to different reflecting optics configurations. It has been mounted on an asymmetrical parabolic trough concentrator to form a solar collector with a concentration ratio of 42, which has been experimentally investigated. In particular, a new test procedure is presented, applied and validated to characterize the thermal performance of the collector during steam generation. The results show that a promising overall thermal efficiency of 64% at $0.160\,K\,m^2\,W^{-1}$ can be achieved with negligible pressure drop.

17/01851 Numerical study of a tangentially fired boiler for reducing steam tube overheating

Tang, G. *et al. Applied Thermal Engineering*, 2016, 102, 261–271.

A comprehensive numerical and experimental study on a 200 MW tangentially fired boiler firing metallurgical gases was conducted. A three-dimensional computational fluid dynamics model was developed to simulate the flow characteristics and combustion process inside the boiler. The eddy dissipation concept combustion model was applied to take into account detailed turbulent interactive reacting chemical reactions. Field experiments were also conducted on the original tangentially fired boiler under different operation conditions. Flame profiles videos were captured during experiments. A quick comparison of the experimental flame profile with numerical simulation results shows good agreement. Wall steam tubes overheating problem was observed, and the hot spots were identified based on a wide range of typical operation conditions. The effect of total fuel input and natural gas percentage on the furnace wall temperature were investigated.

17/01852 Online optimal control schemes of inlet steam temperature during startup of steam turbines considering low cycle fatigue

Zhang, H. *et al. Energy*, 2016, 117, 105–115.

Great thermal stresses and fatigue damages will be developed during the start-up of steam turbines, which will threaten the safety of operation. To save energy and improve the flexibility of the power unit, inlet steam temperature of steam turbines should be controlled online in an optimal way. A new method to obtain online optimal control schemes of the inlet steam temperature considering low cycle fatigue is presented in this paper using Green's function method and Pontryagin's maximum principle. New analytical models of temperature and thermal stresses are proposed. For a hot start-up, constant material properties are used and the steam temperature history that can maintain maximum von Mises stress close to the permitted value is proved to be the optimal control scheme. For a cold or warm start-up, the optimization thermal stress considering temperature dependent material properties is found to be determinated by material properties and Green's functions, which may not be equal to the maximum permitted value. Application of the proposed method to the cold start-up process of a 600 MW steam turbine is introduced. Compared with the conventional start-up scheduling, the proposed optimal control scheme can shorten the time of start-up greatly without exceeding permitted fatigue damage.

17/01853 Polymer heat exchanger design for condensing boiler applications

Trojanowski, R. *et al. Applied Thermal Engineering*, 2016, 103, 150–158.

Condensing boilers achieve very high efficiency levels by recovering both sensible heat and water vapour latent heat from the flue gas. Research since the 1980s has focused on corrosion in such condensing heat exchangers related to the acidic condensate and material selection. Polymers in condensing heat exchangers have been considered to avoid the cost and corrosion concerns of metallic designs. Past efforts have shown that polymers offer the advantage of corrosion resistance and cost, however, lower thermal conductivity limited their application. More recent developments have introduced thermally conductive polymers which now offer promising conductivity values. This project focused on the evaluation of a thermally conductive polymer heat exchanger for this application. Computational fluid dynamic results indicated thermal conductivity values of stainless steel, a typical heat exchanger material, do not need to be achieved for similar heat transfer performance. An increase in thermal conductivity from about 10 times that of the base polymer can achieve an overall heat exchanger effectiveness similar to that achieved with stainless steel. A polymer composite thermal conductivity of approximately $2.5\,W/m\cdot K$ would be adequate. Thermally conductive polymer materials are now commercially available which offer values up to $20\,W/m\cdot K$. In this work, one Nylon-12 and one thermally conductive polymer composite heat exchanger prototypes were constructed for a condensing boiler application. Tests demonstrated that good overall heat transfer performance was achieved. The lower thermal conductivity of the polymer heat exchanger will lead to higher surface temperatures and lower water condensation rates.

17/01854 Reduction of main steam temperature deviation in a tangentially coal-fired, two pass boiler

Park, H. Y. *et al. Fuel*, 2016, 166, 509–516.

This paper describes the main steam temperature deviation and its reduction by changing the injection angles of over-fire air in a 800 MW, tangentially coal-fired, two pass boiler. The computational fluid dynamics (CFD) simulation showed that the simulated gas temperatures and velocities in the furnace are well matched with the steam temperatures along the steam pathways and the tube metal temperatures of the heaters. The changes in injection angles of over-fire air clearly affect the temperature and flow fields in front of the final superheater, in turn, the main steam temperatures at the final superheater outlet. With the findings of the CFD simulation and the relevant plant data, the field tests to reduce the deviation were performed by changing the yaw and tilt angles of separate over-fire air (SOFA) and closed coupled over-fire air (CCOFA). The field tests showed that, under the optimized injection angles of SOFA and CCOFA, the main steam temperature deviation was reduced from 27 to 9 °C and the reheat steam temperature was increased to the desired value.

17/01855 Relations for steam power plant condenser performance in off-design conditions in the function of inlet parameters and those relevant in reference conditions

Laskowski, R. *Applied Thermal Engineering*, 2016, 103, 528–536.

In the classical approach, the effectiveness of a steam power plant condenser, being a surface-type steam–water heat exchanger, can be given as a function of an overall heat transfer coefficient, heat transfer surface area, cooling water mass flow rate, and the specific heat of water. The calculation of the overall heat transfer coefficient requires additional equations to determine the overall heat transfer coefficient from steam and water as well as Nusselt, Reynolds, and Prandtl similarity numbers. Basic geometric data of the condenser, such as tube diameter, tube wall thickness, heat exchanger length, and pitch of the tubes, also have to be taken into account. Complete geometric data of a heat exchanger are not always available, which raises further difficulties in developing a model. Hence, it is justified to provide a single equation for the steam power plant condenser effectiveness in off-design conditions (without any additional heat transfer equations) as a function of three independent parameters, such as cooling water temperature at the inlet, cooling water mass flow rate, and steam temperature, along with corresponding reference parameters (relevant under nominal operating conditions). The paper formulates two simplified equations for the steam power plant condenser effectiveness and the cooling water outlet temperature as functions of the parameters and reference conditions mentioned above. The proposed relations were verified against data obtained using a steam condenser simulator (written in Fortran), actual measurement data from a power plant, and measurement data available in the literature. One of the proposed relations is explicit but its use is limited to the range of number of transfer units (NTU) between 0.5 and 1.5. The other one is not limited to any range of NTU, but is an implicit function and has to be solved in an iterative process. The data obtained using the steam condenser simulator, actual measurement data, and data available in the literature allow the conclusion that the proposed equations provide good accuracy.

17/01856 Sensitivity study of APR-1400 steam generator primary head stay cylinder and tube sheet thickness

Abdallah, K. A. A. and Namgung, I. *Annals of Nuclear Energy*, 2016, 92, 8–15.

The steam generator is a type of heat exchanger which produces steam to drive the turbine generator. For the APR-1400, Doosan Heavy Industries & Construction manufactures a vertical type of steam generator that has a horizontal tube sheet with a central support design, called a stay cylinder. In this design, the stay cylinder limits

tube sheet deformation and effectively reduces thickness of tube sheet and increases structural integrity. A concentric hole in the stay cylinder facilitates welding to the primary head and to the tube sheet. In this study, the APR-1400 steam generator tube sheet thickness parameters were investigated within the constraint of maintaining the overall deformation of the tube sheet in comparison to the current design. A parametric evaluation to reduce the thickness of the steam generator tube sheet is performed by varying the inner diameter of the stay cylinder and the thickness of the tube sheet. The solutions are developed based on two-dimensional finite element analyses. The effect of a reduction of the tube sheet is beneficial in the manufacturing of steam generator by using less material and reducing manufacturing time and allowing easier assembly process of U-tube bundles to the tube sheet.

17/01857 Studies on heat flux distribution on the membrane walls in a 600 MW supercritical arch-fired boiler
Zhang, D. *et al. Applied Thermal Engineering*, 2016, 103, 264–273.
The heat flux distributions on the membrane walls in the furnace of a 600 MW supercritical arch-fired boiler (SC-AFB) were studied by numerical simulation and field measurements. The results revealed that on the front and rear walls, the horizontal heat flux profiles in the upper furnace exhibit an M-shaped pattern. At full boiler load, on the front wall the distance between two peaks is about half of the furnace width around the conjunction area of the upper and lower furnaces and it decreases as the furnace height increases. While on the rear wall, the two high heat flux zones on each half wall nearly merge and the distance between the two peaks is about one-third of the boiler width. As boiler load decreases, the heat flux is smaller and distribution becomes more uniform. At all loads, on the side walls, the profiles are only in bell-shaped. The predicted heat flux distributions are in good agreement in trend and value with the measurement data. Numerical simulation also revealed that the M-shaped heat flux distribution is a special feature of an AFB/SC-AFB whose furnace has a rectangular horizontal cross section with a large width/depth ratio. Some suggestions are provided to improve the aerodynamics field and combustion in the SC-AFBs.

17/01858 Techno-economic comparison of boiler cold-end exhaust gas heat recovery processes for efficient brown-coal-fired power generation
Ma, Y. *et al. Energy*, 2016, 116, 812–823.
An important way to increase power plant thermal efficiency is to recover exhaust gas heat at the boiler cold-end with the stepwise integration of a steam turbine heat regenerative system. To this end, there are currently three typical heat recovery processes, i.e. a low-temperature economizer (LTE), segmented air heating (SAH) and bypass flue (BPF), for recovery. To provide useful guidance to thermal power plants for optimal and efficient processes, the thermal economy and techno-economic performance of the three aforementioned processes were calculated and compared using an in-service 600 MW brown-coal-fired supercritical power unit as a reference. The results demonstrate that with the use of these three processes, the net standard coal consumption rate of the unit can be reduced by 4.43, 5.84 and 6.48 g/(kW h); meanwhile, 3.84, 3.52 and 3.39 million US dollars are the initial costs of the three heat recovery projects. If the 600 MW unit runs 5500 h per year at the rated load, the three processes can annually increase the earnings of the unit by 1.49, 2.03 and 2.27 million US dollars from coal savings, meaning that their dynamic payback periods are 3.12, 2.00 and 1.71 years, respectively. The results indicate that for a brown-coal-fired power unit, the coal savings achieved by exhaust heat recovery are significant. In comparison with the conventional LTE, SAH shows an improvement in thermal economy and techno-economic performance, but it currently faces difficulties in engineering applications. Among the three processes, the BPF shows the best thermal economy and techno-economic performance, as well as good engineering feasibility; therefore, it is recommended for application.

08 COMBUSTION

Burners, combustion systems

17/01859 A funnel plot to assess energy yield and oil quality for pyrolysis-based processes
DeSisto, W. J. and Wheeler, M. C. *Biomass and Bioenergy*, 2016, 93, 254–258.
The conversion of biomass to hydrocarbon transportation fuels presents unique challenges that generally focus on maintaining high mass and energy yields while removing oxygen from the biomass. Among the many processes proposed and demonstrated, processes that can achieve this efficiently and economically will have a clear advantage. Currently, there is no graphical method to analyse such conversion processes. In this work, a funnel plot was introduced to indicate both product quality, in terms of oxygen removal, and energy yield, the energy retained in the product oil from the original biomass. The funnel plot is applied to literature data for several processes and compared to an idealized chemical conversion of biomass revealing some of the current challenges associated with biofuel production.

17/01860 Catalytic combustion of sulphur-containing methane lean emissions in a reverse-flow reactor with integrated adsorption
Urbani, C. *et al. Chemical Engineering Journal*, 2016, 285, 39–48.
Lean methane emissions (0.15–0.5% CH_4) often contain low concentrations of sulfur compounds (e.g. H_2S). Regenerative catalytic oxidation is an efficient process for methane removal and upgrading of these streams, but the presence of sulfur compounds deactivates typical combustion catalysts. In this work a new strategy is proposed for overcoming this problem, by using a reverse flow reactor provided with integrated adsorption beds. Therefore, it is possible to operate autothermically with low methane concentrations, as well as effectively separate the sulfur compounds before reaching catalytic bed. The working principle of this device has been experimentally demonstrated in a bench-scale reactor working at conditions typical for industrial emissions (GHSV = 1146 h^{-1}, 4300 ppm CH_4, 100–500 ppm H_2S). It has been found that molecular sieve 5A is a suitable adsorbent for this device. The influence of the main reverse flow reactor variables, switching time (200–400 s) and methane feed concentration (4000–4500 ppm), on the performance of the process has been studied. The integrated adsorption performs better at switching time 400 s, while methane concentration has negligible influence, provided that the reactor is maintained ignited.

17/01861 Combustion of coal mine ventilation air methane in a regenerative combustor with integrated adsorption: reactor design and optimization
Fernández, J. *et al. Applied Thermal Engineering*, 2016, 102, 167–175.
Coal mine ventilation air methane is an important environmental concern due to its contribution to global warming. Catalytic combustion in reverse flow reactors is an efficient treatment technique, but high emission moistures lead to catalyst inhibition. To overcome this issue a novel reverse flow reactor with integrated water adsorption has been proposed. In this work, the design of a reverse flow reactor adequate to treat a typical real coal ventilation stream, 45 m^3/s with 0.30% (mol) methane and 5% (mol) water, has been studied. The performance of the reactor design has been simulated using a 1D heterogeneous dynamic model, previously validated with experimental results. Particular attention has been paid to reactor stability when water and methane feed concentration change upon time. Real coal mine ventilation air data have been used to produce realistic simulations. The optimization of the operating conditions (surface velocity and switching time) has been carried out based on the total cost of the reactor (considering fixed capital and 10-year variable cost).

17/01862 Design of a partially aerated naturally aspirated burner for producer gas
Sutar, K. B. *et al. Energy*, 2016, 116, 773–785.
This article presents a detailed methodology for the design of a partially aerated naturally aspirated burner used for combustion of the producer gas generated in a downdraft gasifier cookstove. The main difference between an liquid petroleum gas burner and producer gas burner is that the former uses a high-velocity jet of gas at ambient temperature whereas the latter uses a low velocity, high mass flow rate, buoyant jet of gas at 100–300 °C. Due to the elevated temperatures, buoyancy force plays an important role in entraining combustion air into the burner for producer gas. This has been accounted for in the new methodology, developed based on the design procedure available in the literature for hydrocarbon fuels. A mathematical model for fluid flow and heat transfer through the burner has been developed to predict percentage of primary aeration in the burner at different producer gas flow rates. The pressure drops predicted by the model have been validated using experimental measurements. The predictions of the model have been used to corroborate the assumptions and heuristics used in the design methodology. The predictions have also been used to demonstrate the importance of considering buoyancy in burner design, by comparing with a burner designed ignoring buoyancy. With the use of the newly designed burner, the thermal efficiency of the gasifier cookstove was found to improve substantially. Carbon monoxide emissions from the cookstove using this burner were also found to be within the limits (<5 g/MJ_d) recommended in the Indian standards for cookstoves.

17/01863 Detailed kinetic mechanism of gas-phase reactions of volatiles released from biomass pyrolysis

Debiagi, P. E. A. *et al. Biomass and Bioenergy*, 2016, 93, 60–71.

Comprehensive chemical models to describe the behaviour of biomass pyrolysis, gasification and combustion are crucial for the simulation and design of thermochemical processes of lignocellulosic materials. Despite this importance, reliable and predictive models are still not well known. The original aspect of this work is to present a comprehensive and predictive model of pyrolysis, gasification, and combustion, starting from biomass characterization, through the description of released volatiles at the particle scale, until the effect of the secondary gas-phase reactions at the reactor scale. All these aspects can play a relevant role in the biomass thermo-valorization processes. Most of released species from biomass devolatilization are oxygenated hydrocarbons. This study aims at identifying some reference rate parameters, based on analogy and thermochemistry rules, for the different reaction classes. Once rate rules are defined, they allow an easy extension to analogous compounds. In this way, the kinetic mechanism already developed for jet and diesel fuels is extended to the new tar species released by biomasses. Despite unavoidable approximations when the interest is also at the reactor scale, this model is the only one, to the authors' knowledge, able to describe the whole process from biomass to final products, in a predictive and satisfactory way.

17/01864 Investigations on the effect of methanol blend on the combustion parameters of dual fuel diesel engine

Prashant, G. K. *et al. Applied Thermal Engineering*, 2016, 103, 187–194.

Ignition delay, maximum rate of pressure rise, heat release rate, temperature and cylinder peak pressure of a four-cylinder (turbo-charged and intercooled) 62.5 kW gen-set diesel engine using methanol blend were experimentally investigated. When the amount of methanol in diesel fuel is increased, the ignition delay increases as compared to pure diesel operation. It is found that the maximum rate of pressure rise were found to increase (3.1%, 14.6% and 19.5% at 10%, 20% and 40% load conditions) along with the peak pressure rise (2.5% and 9.5% at 10% and 20% load conditions) compared to diesel operation. While ignition delays observed for mixture of 20% methanol were found to decrease (by 5° CA), respectively. The minimum and maximum net heat release rates were found to be 35.93 and 78.07 kJ (40% mixture of methanol at 40% and 10% load conditions). Three factor analysis of the rate of pressure rise, net heat release, cumulative heat release and ignition delay were in agreement of the experimental results.

17/01865 Non-isothermal pyrolysis of de-oiled microalgal biomass: kinetics and evolved gas analysis

Maurya, R. *et al. Bioresource Technology*, 2016, 221, 251–261.

Non-isothermal ($\beta = 5$, 10, 20, 35 °C/min) pyrolysis of de-oiled microalgal biomass (DMB) of *Chlorella variabilis* was investigated by TGA-MS (30–900 °C, argon atmosphere) to understand thermal decomposition and evolved gas analysis (EGA). The results showed that three-stage thermal decomposition and three volatilization zone (100–400, 400–550 and 600–750 °C) of organic matters during pyrolysis. The highest rate of weight-loss is 8.91%/min at 302 °C for 35 °C/min heating-rate. Kinetics of pyrolysis were investigated by iso-conversional (KAS, FWO) and model-fitting (Coats–Redfern) method. For Zones 1 and 3, similar activation energy (E_a) is found in between KAS ($\alpha = 0.4$), FWO ($\alpha = 0.4$) and Avrami–Erofe'ev ($n = 4$) model. Using the best-fitted kinetic model Avrami–Erofe'ev ($n = 4$), E_a values ($R^2 = > 0.96$) are 171.12 (Zone 1), 404.65 (Zone 2) and 691.42 kJ/mol (Zone 3). EGA indicate the abundance of most gases observed consequently between 200–300 and 400–500 °C. The pyrolysis of DMB involved multi-step reaction mechanisms for solid-state reactions having different E_a values.

17/01866 Numerical simulation of oxy-coal combustion in a rotary cement kiln

Wang, M. *et al. Applied Thermal Engineering*, 2016, 103, 491–500.

In this paper, a comprehensive computational fluid dynamics (CFD) methodology was adopted to investigate the characteristics of oxy-coal combustion in a cement kiln with a specially designed burner. The simulation was conducted under five oxidant stream conditions with different O_2/N_2 volume ratios: 21/79, 24/76, 27/73, 30/70, and 33/67. The results revealed that there is strong entrainment from the primary air to the secondary air, resulting in an inner recirculation zone and outside recirculation zone. The oxygen-enriched combustion increases the maximum temperature and improves the combustion efficiency; however, the uniformity of the temperature field becomes worse. The temperature rises sharply as the oxygen content increases; however, the enhancement is slight when the oxygen content exceeds 30%. At a lower oxygen content (<27%), the NO_x emissions increase slowly as the oxygen content increases, whereas NO_x increases sharply when the oxygen content exceeds 27% in volume. This suggests that the optimal oxygen content is no more than 27% for pulverized coal combustion in a cement kiln. The simulation results reasonably agree with the measured data. The findings of this work will help save fuel consumption and decrease production cost.

17/01867 Oxy-combustion of coal, lignite and biomass: a techno-economic analysis for a large scale carbon capture and storage (CCS) project in Romania

Cormos, C.-C. *Fuel*, 2016, 169, 50–57.

Oxy-fuel combustion is a promising power generation technology for reducing both energy and cost penalties for CO_2 capture. This paper presents a detailed techno-economic analysis for oxy-combustion power plant to generate about 350 MW net power with a carbon capture rate higher than 90%. Both fossil fuels (coal and lignite) and renewable energy sources (sawdust) were used to fuel a super-critical power plant (live steam parameters: 582 °C/29 MPa). The assessment is based on numerical analysis, the models of various power plant sub-systems being built in ChemCAD and Thermflow software. As benchmark option used to quantify the CO_2 capture energy and cost penalties, the same super-critical power plant without CCS was considered. The investigated coal, lignite and sawdust oxy-combustion cases show an energy penalty of 9–12 net efficiency percentage points, 37–50% increase of total capital investment, the O&M costs are increasing with 7–15% and the electricity cost with 54–95% (all compared to coal-fuelled non-CCS case). Sensitivity studies were also performed to evaluate the influence of various economic parameters on electricity and CO_2 avoidance costs.

17/01868 Oxygen enriched combustion and co-combustion of lignites and biomass in a 30 kWth circulating fluidized bed

Kayahan, U. and Özdoğan, S. *Energy*, 2016, 116, 317–328.

Oxygen-enriched combustion is a promising retrofitting option for existing power plants to improve CO_2 capture. In this study, the effect of oxygen enrichment of air as oxidant was investigated with a 30 kWth fluidized bed combustor. Tests were conducted with two different Turkish lignites, one biomass and their blends. Biomass share was increased up to 20%. The oxygen concentration in the oxidant was kept between 21% and 30%. Oxygen enrichment supports combustion in all cases. Biomass addition to lignites appears to have an increasing synergetic effect on combustion as the oxygen enrichment and biomass portion in the mix increases. It was found that oxygen enrichment increases NO and SO_2 formation in all cases. As the biomass share increases NO emissions increase in all oxygen cases while the opposite is true for SO_2 emissions.

17/01869 Propagation characteristics of laminar spherical flames within homogeneous hydrogen-air mixtures

Sun, Z.-Y. and Li, G.-X. *Energy*, 2016, 116, 116–127.

Taking the laminar spherical flames propagate within homogenous hydrogen–air mixture as the studied object, the effects of initial conditions (including equivalence ratio, initial pressure, and initial temperature) on propagation characteristics are systematically investigated. During propagation, global stretch rate monotonously declines towards convergence, it first rises then declines with the increase of equivalence ratio (φ) from 0.5 to 4.0 and the maximal value is attained at $\varphi = 1.8$. With the declines of global stretch rate, the propagation speed within lean mixtures first declines and then rises, but it monotonously rises within stoichiometric and rich mixtures. Markstein length is sensitive to equivalence ratio and initial pressure rather than initial temperature. Unstretched laminar burning velocity is not monotonously changed with the variation of equivalence ratio but it monotonously verifies with the variation of initial thermodynamic condition. Owing to the wane of stretch effects, flame develops towards unstable, the nexus between critical flame radius of cellularity behaviours and initial conditions are analysed based upon hydrodynamic and thermal-diffusive effects. In addition, the critical Peclet number is observed linear to equivalence ratio but less sensitive to initial ambient conditions.

17/01870 Pyrolysis kinetics and behavior of potassium-impregnated pine wood in TGA and a fixed-bed reactor

Guo, F. *et al. Energy Conversion and Management*, 2016, 130, 184–191.

Potassium is a well-known alkali catalyst in the thermal reactions of biomass. The effect of potassium on the pyrolysis behaviour and kinetics of biomass was investigated through thermogravimetric analysis (TGA) and a fixed bed in this study. The addition of potassium reduced initial and peak temperature in TGA curves, promoting the decomposition process of biomass. The effect of potassium on the apparent activation energy varies at different conversion degree (a) and lower apparent activation energy was obtained at the initial stage ($a \leq 0.3$) of the pyrolysis process. The influence of potassium on the volatiles releasing behaviour was dependent on the amount of loading potassium. The gas yield was significantly increased with the increasing of potassium concentration when the impregnated potassium was below 0.3 mol/kg. Particularly, the yield of H_2 and CO_2 was promoted by potassium. Higher potassium content may contribute to the increase

in reactivity towards tar molecules, leading to quickly decrease in tar yield. The surface chemical characteristics of char were determined by Fourier transform infrared spectroscopic method. Above a certain threshold surface concentration of potassium, scanning electron microscopy analysis shows that agglomeration is a potential threat at high temperature, which can block the active sites and decrease the activity during biomass thermal decomposition.

17/01871 Pyrolysis of eastern redcedar: distribution and characteristics of fast and slow pyrolysis products

Yang, Z. *et al. Fuel*, 2016, 166, 157–165.

Eastern redcedar is a problematic plant in Oklahoma due to its extinguished environmental flexibility and rapid expansion. Thermally converting solid biomass polymers into liquid fuel intermediate, solid char and gaseous products through pyrolysis is one promising approach to use redcedar for the production of sustainable fuels. The objective of this study was to investigate effects of eastern redcedar wood zones (heartwood and sapwood), pyrolysis temperature (450 and 500 °C) and pyrolysis types (slow at lab-scale and fast at micro-scale) on the distribution and composition of the pyrolysis products. In fast pyrolysis conditions, the products were dominated by anhydrous sugars, phenols and guaiacols. The total yield of lignin-derived compounds from heartwood was higher than that from sapwood at 500 °C but the total yields were not significantly different at 450 °C. In slow pyrolysis conditions, acetic acid and furfural were the two most abundant species in bio-oil. Slow pyrolysis products consisted of less branched compounds of phenols and guaiacols as compared to fast pyrolysis products. Cedar oil components (alpha/beta-cedrene) were only produced at slow pyrolysis conditions and its maximum yield (21.04 ± 1.08 area%) of was obtained from heartwood at 500 °C. Heartwood produced significantly more cedrenes than sapwood.

17/01872 Pyrolysis of hornbeam (*Carpinus betulus* L.) sawdust: characterization of bio-oil and bio-char

Morali, U. *et al. Bioresource Technology*, 2016, 221, 682–685.

Slow pyrolysis of hornbeam (*Carpinus betulus* L.) sawdust was performed to produce bio-oil and bio-char. The operational variables were as follows: pyrolysis temperature (400–600 °C), heating rate (10–50 °C min^{-1}) and nitrogen flow rate (50–150 cm^3 min^{-1}). Physicochemical and thermogravimetric characterizations of hornbeam sawdust were performed. The characteristics of bio-oil and bio-char were analysed on the basis of various spectroscopic and chromatographic techniques such as FTIR, GC–MS, 1H NMR, SEM, BET. Higher heating value, density and kinematic viscosity of the bio-oil with maximum yield of 35.28% were 23.22 MJ kg^{-1}, 1289 kg m^{-3} and 0.6 mm^2 s^{-1}, respectively. The bio-oil with relatively high fuel potential can be obtained from the pyrolysis of the hornbeam sawdust and the bio-char with a calorific value of 32.88 MJ kg^{-1} is a promising candidate for solid fuel applications that also contributes to the preservation of the environment.

17/01873 Recent progress on biomass co-pyrolysis conversion into high-quality bio-oil

Hassan, H. *et al. Bioresource Technology*, 2016, 221, 645–655.

Co-pyrolysis of biomass with abundantly available materials could be an economical method for production of bio-fuels. However, elimination of oxygenated compounds poses a considerable challenge. Catalytic co-pyrolysis is another potential technique for upgrading bio-oils for application as liquid fuels in standard engines. This technique promotes the production of high-quality bio-oil through acid catalysed reduction of oxygenated compounds and mutagenic polyaromatic hydrocarbons. This work aims to review and summarize research progress on co-pyrolysis and catalytic co-pyrolysis, as well as their benefits on enhancement of bio-oils derived from biomass. This review focuses on the potential of plastic wastes and coal materials as co-feed in co-pyrolysis to produce valuable liquid fuel. This paper also proposes future directions for using this technique to obtain high yields of bio-oils.

17/01874 Sooting tendency and particle size distributions of n-heptane/toluene mixtures burned in a wick-fed diffusion flame

Botero, M. L. *et al. Fuel*, 2016, 169, 111–119.

The sooting characteristics of binary mixtures of n-heptane and toluene and a commercial gasoline were studied. The experiment involves the non-premixed combustion of the fuel in wick-fed burner. The particle size distributions (PSDs) of soot were measured at the tip of flames of different heights, using a differential mobility spectrometer. Transmission electron microscopy was used to investigate the morphology of the particles formed. Pure n-heptane and toluene were studied along with blends of 10%, 30%, and 50% by volume of toluene in n-heptane. The addition of toluene to heptane shifts the PSD to larger diameters. As toluene is added to n-heptane the dependence of soot particle size on flame height changes from resembling a paraffinic to resembling an aromatic fuel in a non-linear fashion. A tolerance to toluene addition at the lowest flow rates was found, where particles were not detected. A commercial gasoline with approximately 44% by mass of aromatics was also analysed. The smoke point and PSDs are similar to the mixture 50% toluene 50% n-heptane, but the mean aggregate mobility size, number of particles and primary particle size formed by the gasoline are smaller.

17/01875 Spectral characteristics of a premixed oxy-methane flame in atmospheric conditions

Oh, J. *Energy*, 2016, 116, 986–997.

The characteristics of light emission of a premixed oxy-methane flame were experimentally investigated in atmospheric conditions ($T_\infty = 24$ °C and $P_\infty = 1.01325$ bar). The objectives of the current study are to investigate the flame luminescence and flame spectra of a premixed oxy-methane flame in a cylindrical tube burner and to derive an empirical formula describing the relationship between chemiluminescence intensity ratio, fuel flow rate, global equivalence ratio, and diluent mole fraction. The mixture velocity at nozzle exit (u_o) was varied in u_o = (15–35) m/s and the global equivalence ratio (ϕ_G) was changed from 0.4 to 2.0 with a cylindrical tube burner of $d_o = 2.03$ mm. A spectrometer and intensified charge-coupled device camera were used to detect flame chemiluminescence with narrow band-pass filters and lenses. The light emission of a laminar premixed oxy-methane flame was more dominant at $\lambda = 308$ nm than at other wavelengths from the measurement of spectral intensity. The intensity of OH* and CH* increased with an increase in mass flow rate of fuel (m_F), adiabatic flame temperature (T_{Ad}), and equivalence ratio (ϕ_G) in $\phi_G = 0.5$–1.1. The intensity ratio of OH*/CH* was expressed as a function of the fuel flow rate, equivalence ratio, and diluent mole fraction (X_D).

17/01876 State-of-the-art in premixed combustion modeling using flamelet generated manifolds

van Oijen, J. A. *et al. Progress in Energy and Combustion Science*, 2016, 57, 30–74.

Flamelet based chemical reduction techniques are very promising methods for efficient and accurate modelling of premixed flames. Over the years the flamelet generated manifold (FGM) technique has been developed by the Combustion Technology Group of Eindhoven University of Technology. Current state-of-the-art of FGM for the modelling of premixed and partially-premixed flames is reviewed. The fundamental basis of FGM consists of a generalized description of the flame front in a (possibly moving) flame-adapted coordinate system. The basic nature of the generalized flamelet model is that effects of strong stretch in turbulent flames are taken into account by resolving the detailed structure of flame stretch and curvature inside the flame front. The generalized flamelet model, which forms the basis on which FGM is built, is derived in Part I. To be able to validate numerical results of flames obtained with full chemistry and obtained from FGM, it is important that the generalized flamelet model is analysed further. This is done by investigating the impact of strong stretch, curvature and preferential diffusion effects on the flame dynamics as described by the local mass burning rate. This so-called strong stretch theory is derived and analysed in Part I, as well as multiple simplifications of it, to compare the strong stretch theory with existing stretch theories. The results compare well with numerical results for flames with thin reaction layers, but described by multiple-species transport and chemistry. This opens the way to use the generalized flamelet model as a firm basis for applying FGM in strongly stretched laminar and turbulent flames in Part II. The complete FGM model is derived first and the use of FGM in practice is reviewed. The FGM model is then validated by studying effects of flame stretch, heat loss, and changes in elements, as well as NO formation. The application to direct numerical simulations of turbulent flames is subsequently studied and validated using the strong stretch theory. It is shown that the generalized flamelet model still holds even in case of strong stretch and curvature effects, at least as long as the reaction layer is dominated by reaction and diffusion phenomena and not perturbed too much by stretch related perturbations. The FGM model then still performs very well with a low number of control variables. Turbulent flames with strong preferential diffusion effects can also be modelled efficiently with an FGM model using a single additional control variable for the changes in element mass fractions and enthalpy. Finally FGM is applied to the modelling of turbulent flames using LES and RANS flow solvers. For these cases, the flame front structure is not resolved anymore and unresolved terms need to be modelled. A common approach to include unresolved turbulent fluctuations is the presumed probability density function (PDF) approach. The validity of this FGM-PDF approach is discussed for a few test cases with increasing level of complexity.

17/01877 Study of a new combined method for pre-extraction of essential oils and catalytic fast pyrolysis of pine sawdust

Ming, Z.-Q. *et al. Energy*, 2016, 116, 558–566.

A new combined method for the pre-extraction of essential oils (EOs) and the uniformly dispersion of alkaline earth metal oxide (AEMO) on pine sawdust (PS) was investigated. EOs were firstly extracted from PS after mixing with a certain amount of AEMO through steam distillation (SD), and then the pretreated PS was utilized in the process of fast pyrolysis to produce the upgraded bio-oil. A maximum extraction yield of EOs was 1.61 wt% from PS mixed with 5 wt% CaO within 300 min, compared with 1.21 wt% from the control (raw PS). The proportion of alcohols in EOs increased significantly when using PS mixed with AEMO. When PS was pretreated by the combined AEMO mixing and SD, the content of hydrocarbons in organic phase of the bio-oil increased significantly while that of acids and $C_nH_mO_x$ decreased. The analysis of physicochemical properties for the bio-oil further demonstrated that the quality of bio-oil was improved based on the new pretreatment method. Furthermore, the maximum bio-oil yield was obtained at pyrolysis temperature of 500 °C in almost all cases.

17/01878 Thermal properties and energetic characteristics of a combustion system

Fu, X. Q. *et al. Applied Thermal Engineering*, 2016, 103, 874–882.

In this paper, the thermal decomposition characteristics and the energy characteristics were studied to select a suitable propellant formulation. The temperature distribution of micro-thruster array was calculated to study the effect of heat loss on the combustion chamber shell. The monopropellant micro motor model was established, and the effect of heat loss on the micro-thruster performance was studied. Results indicated that 5 : 5 lead styphnate/nitrocellulose was suitable as micromotor formulation, and the highest temperature appeared at the boundary of the combustion chamber, where the thermal stress and deformation were the maximum. Furthermore, the thermal stress and deformation of silicon material was smaller than steel and the thermal stress was the main reason for the destruction of microthruster stability. In addition, the heat loss had great effects on microthruster performance: the thrust decreased by 21.7%, and the specific impulse also decreased by 11.8%.

Fire safety

17/01879 Atmospheric occurrence and fate of organophosphorus flame retardants and plasticizer at the German coast

Wolschke, H. *et al. Atmospheric Environment*, 2016, 137, 1–5.

This study reports the occurrence and distribution of organophosphor esters (OPEs), used as flame retardants and plasticizer, in the marine atmosphere of the German coast. From August 2011 to October 2012, 58 high volume air samples (gas/particle phase separately) were collected at the German North Sea coast town Büsum. With the use of a GC-MS/MS system for instrumental analysis, detection limits for OPEs in air samples could be significantly improved compared to the previously used single GC-MS method. The concentration (gas + particle phase) of total OPEs was on average 5 pg/m^3, with eight of the nine investigated compounds detectable in over 50% of the samples. A focus of this investigation concerned the partioning of OPEs between the particle and the gas phase. The observed partitioning of OPEs in this study was distinguished from previous studies. While previous studies reported OPEs exclusively in the particle phase, a significant part of the sum OPE concentration (55%) was detected in the gas phase. The contribution of the gas phase even reached up to as high as 88% for individual compounds such as tri-iso-butyl phosphate.

17/01880 Fire risk analysis based on one-dimensional model in nuclear power plant

Yu, Y. *et al. Annals of Nuclear Energy*, 2016, 94, 409–414.

Fire probabilistic safety assessment (fire PSA) is developed to give the insight of nuclear power plant risk induced by fire accident and the main contributors, and fire accident scenario analysis is one of the important parts in the work to get the key factors such as time to target damage and time to detection. The thermal–hydraulic model simulating fire accident should have enough accuracy and high speed to satisfy the request of fire PSA. Many researches indicate that in a large volume the hot fluid will concentrate in the upper part while the cold fluid will be in the lower part because of density difference under fire condition, that is, the gradients of temperature and of some other parameters in vertical direction are much greater than in horizontal direction. Based on such thermal stratification theory a one-dimensional model is developed, and the buoyant jet is used to simulate the process of heated air flowing up. In this paper a fire in a compartment is analysed based on one-dimensional model and the temperature distribution is obtained, the results are compared with those of commercial software such as FDT, CFAST and FDS, then the time to target damage is evaluated based on results of different models and the fire non-suppression probabilities are evaluated. The results illustrate that one-dimensional model has better accuracy than FDT and CFAST since such a model can simulate the thermal stratification and natural circulation which exist in the volume simultaneously. Moreover when the fire power is low, the thermal stratification is apparent and air temperature in the hot upper layer is much lower than the critical value of target damage, the one-dimensional model has enough accuracy to be used directly in fire PSA. While the thermal stratification will be weakened when the fire power increases because of the effects of radiation heat transfer and the entrainment by the jet, so more detailed model such as FDS is needed for such situations, however the results of one-dimensional model can give the advice for the proper simulation time of FDS to improve the calculation efficiency when the upper part temperature is close to or higher than the critical value.

17/01881 Hydrogen risk for advanced PWR under typical severe accidents induced by DVI line break

Tong, L. L. *Annals of Nuclear Energy*, 2016, 94, 325–331.

Advanced passive pressurized water reactor (APWR) relies on in-vessel retention (IVR) of molten core debris under severe accidents, which makes hydrogen generation and distribution different with other PWRs. Hydrogen generation and hydrogen risk for APWR is studied with the integrated severe accident plant model, including reactor coolant system (RCS), engineered safety features (ESFs), simplified secondary side, containment and passive containment cooling system (PCCS). Initial events of DVI line break with passive core cooling system (PXS) compartment not flooded (named Case 1), DVI line break with PXS compartment flooded through broken DVI line (named Case 2), and DVI line break with IRWST direct injection available based on Case 1 (named Case 3) are selected to study hydrogen generation in pressure vessel, distributions in containment, and hydrogen risk controlled with igniters. Results show that hydrogen generated in pressure vessel is 257, 461 and 499 kg for Case 1 to Case 3 due to different thermal hydraulic characteristics. During maintaining the water level in the pressure vessel with the safety measures, zirconium–steam reaction is violent and the duration of hydrogen generation is longer than the other two cases due to the availability of plenty of steam, resulting in an amount of hydrogen generation, and hydrogen distribution in upper containment is nearly 10%. Case 3 is screened to analyse the effectiveness of hydrogen control system consisting of igniters, showing that the hydrogen control system can mitigate hydrogen risk when igniters are available at the SAMG inlet condition.

17/01882 On the determination of the mesh size for numerical simulations of shock wave propagation in near field underwater explosion

Wang, G. *et al. Applied Ocean Research*, 2016, 59, 1–9.

It is well known that the accuracy of mesh-based numerical simulations of underwater explosion strongly relies on the mesh size adopted in the analyses. Although a numerical analysis of underwater explosion can be performed with enough accuracy by using considerably fine meshes, such fine meshes may lead to substantially increase in the CPU time and the usage of computer memory. Thus, how to determine a suitable mesh size in numerical simulations is always a problem confronted when attempting to study the shock wave propagation resulting from underwater explosion and the subsequent response of structures. Considering that there is currently no universally accepted method for resolving this problem, this paper aims to propose a simple method to determine the mesh size for numerical simulations of near field underwater explosion. To this end, the mesh size effects on the shock wave propagation of underwater explosion are carefully investigated for different charge weights, through which the correlation between mesh sizes and charge weights is identified. Based on the numerical study, a dimensionless variable (λ), defined as the ratio of the radius of charge to the side length of element, is introduced to be the criterion for determining the mesh size in simulations. It is interesting to note that the presented method is suitable for various charge weights. By using the proposed meshing rule, adequate balance between solution accuracy and computational efficiency can be achieved for different blast scenarios in numerical simulations of underwater explosion.

09 PROCESS HEATING, POWER AND INCINERATION

Energy applications in industry

17/01883 A comprehensive review on energy efficiency enhancement initiatives in centrifugal pumping system

Shankar, V. K. A. *et al. Applied Energy*, 2016, 181, 495–513.

The energy consumption across the globe is increasing at an alarming rate. This has already shown its impact in the depletion of energy sources and environmental issues (global warming, and weakening of the ozone layer). Certainly, this escalating tendency of energy insufficiency will get aggravated in the future. Efficiency enhancement initiatives are considered to be the key solution in reducing the energy utilization and eventually resisting the global environmental impacts. Of the world's total energy generated, pumping systems, especially the centrifugal pumps consume about 20%. Consequently, the primary focus of global energy policy makers is to enhance energy efficiency in pumping systems. As per the literature, remarkable energy savings can be accomplished by controlling the speed of the pumping system using variable frequency drives (VFDs). For this reason, studies and researches focus primarily on VFD control techniques to improve the efficiency of the pumping system. This article also focuses on component selection, and system dimensioning in addition to the control techniques. Comparison of recent research outcomes of energy efficiency improvements in pumping system has been made to provide an insight for future research.

17/01884 A new search space reduction method based on exergy analysis for distillation columns synthesis

Khalili-Garakani, A. *et al. Energy*, 2016, 116, 795–811.

In distillation process synthesis as the number of components increased, the number of sequences exponentially increased. Besides, there are different categories of sequences which could be considered in the synthesis. So, search space reduction methods are crucial to reduce the number of the candidates and reduce the analysis time. In the present work, a new search space reduction method based on exergy analysis is presented and applied for three different samples of three component mixtures (ESI >1, ESI ≈ 1 and ESI <1). The feed mixture has been tested under three different compositions. The results of the case study were illustrated that the new method could reduce the amount of calculation between 11 and 50%.

17/01885 An MILP model for cost-optimal planning of an on-grid hybrid power system for an eco-industrial park

Theo, W. L. *et al. Energy*, 2016, 116, 1423–1441.

The application of on-grid hybrid power system (HPS) has been effective for harnessing renewable energy resources and ensuring environmental sustainability. A number of algebraic and mathematical modelling approaches have been introduced for the optimization of on-grid HPS. While algebraic power pinch analysis (PoPA) tools have been developed to enable the selection of cost-effective energy storage technology, the available mathematical modelling approaches have yet to consider the economics and storage system selection in the design of an optimal on-grid HPS. This work presents a mixed-integer linear programming (MILP) for the optimal design of an on-grid HPS with the minimum net present value (NPV) of the overall electricity production cost and the selection of the optimum energy storage technology. Two case studies are presented in this work. In the former, the differences between the developed MILP model and previous methods are highlighted, with sensitivity analysis to investigate the impact of electricity tariff on the on-grid HPS. In the second case study, the developed MILP model was applied to an eco-industrial park case study with energy storage technology selection. Lead-acid battery system was found to be the optimal choice due to its low investment requirement.

17/01886 Analysis of the calcium looping system behavior by implementing simple reactor and attrition models at a 10 kW_{th} dual fluidized bed facility under continuous operation

Duelli (Varela), G. *et al. Fuel*, 2016, 169, 79–86.

In this work simplified kinetic and attrition models empirically oriented are implemented in the experimental results of the 10 kW_{th} dual fluidized calcium looping facility at University of Stuttgart. The experimental data used are resulted from continuous operation of a calcium looping facility under conditions close to the industrial ones: wet atmosphere in the carbonator and oxyfired conditions in the regenerator (water vapour presence and high CO_2 volume concentration). The scope of work is to extend the knowledge on the calcium looping systems and to further validate tools which are useful for upscaling purposes as well as for interpretation of experimental results of pilot plants. By using simplified theoretical expressions, the efficiency of the carbonator and the regenerator in terms of CO_2 capture and sorbent calcination conversion respectively is related to the parameter of active space time. The evolution of the particle size of the lime in the course of the process is studied. Fitting constants are applied and a good agreement between the predicted and the actual values of the main process parameters is recorded. The effect of the water vapour presence in both calcination and carbonation reaction is discussed. Results showed CO_2 capture of more than 90% while the carbonator active space time was less than 30 s. Almost full sorbent calcination was recorded while the regenerator active space time was less than 0.11 h. During many hours of carbonator and regenerator operation, a constant particle size of around 400 μm was measured.

17/01887 Application of ARIMA for forecasting energy consumption and GHG emission: a case study of an Indian pig iron manufacturing organization

Sen, P. *et al. Energy*, 2016, 116, 1031–1038.

Environmentally conscious manufacturing (ECM) has become an important strategy and proactive approach for the iron and steel sector of India to produce in an environmentally friendly way and to reduce manufacturing costs. There are several environmentally conscious manufacturing indicators to evaluate ECM programmes. Among those indicators, energy consumption and greenhouse gas (GHG) emissions may be considered critical environmentally conscious manufacturing indicators (CECMI) for the Indian iron and steel sector. This paper focuses on forecasting energy consumption and GHG emissions for an Indian pig iron manufacturing organization because the managers are interested to know the current and future trends of these indicators for better environmental policy. For forecasting purposes, autoregressive integrated moving average (ARIMA) is applied to reveal that ARIMA $(1,0,0)\times(0,1,1)$ is the best fitted model for energy consumption. Regarding GHG emissions, ARIMA $(0,1,4)\times(0,1,1)$ is the best fitted model. In both cases, the forecasts resemble those of the seasonal random trend model, however they appear smoother because the seasonal pattern and the trend are efficiently averaged for energy consumption and as well as GHG emissions. The selection of the correct ARIMA models for these indicators will help in accurate forecasting in order to achieve better environmental management practice.

17/01888 Appropriate placement of vapour recompression in ultra-low energy industrial milk evaporation systems using pinch analysis

Walmsley, T. G. *et al. Energy*, 2016, 116, 1269–1281.

This study focuses on applying pinch analysis to an industrial milk evaporator case study to quantify the potential energy savings. Modern milk evaporators are typically integrated using both mechanical and thermal vapour recompression technologies as the primary means for attaining a high level of energy efficiency. A significant step change in energy efficiency for milk evaporators is achieved in this study by appropriate placement of vapour recompression in a new improved two-effect milk evaporation system design. The grand composite curve helps identify areas for process modifications and placements of vapour recompression that result in energy reduction. In particular, the innovative placement of mechanical vapour recompression in the system unlocks significant energy, energy cost, and emissions savings. The new design requires 78% less steam (6397 kW) at the expense of 16% (364 kW_{ele}) more electricity use. The estimated cost savings associated with the improved design is $942,601/y and the emissions reduction is 3416 t CO_2-e/y. Further energy efficiency improvements and cost savings of $1,411,844/y are gained through improved total site heat integration through recovery of waste heat from the dryer exhaust air and boiler return condensate streams.

17/01889 Automatic derivation of qualitative plant simulation models from legacy piping and instrumentation diagrams

Arroyo, E. *et al. Computers & Chemical Engineering*, 2016, 92, 112–132.

Confronted with the need of plant modernization, facility owners and contractors in the process industry invest significant efforts to create digital plant models allowing for simulation and thereby validation of new engineering solutions. Although an important part of the information required for this task already exists in form of legacy engineering documentation, current computer-aided methods for generating digital plant models cannot exploit this source of knowledge owing to the non-computer-interpretable nature of the available information sources. In an effort to bridge the existing gap, this contribution presents a method based on optical recognition and semantic analysis, which is capable of automatically converting legacy

engineering documents, specifically piping and instrumentation diagrams, into object-oriented plant descriptions and ultimately into qualitative plant simulation models. Resulting simulation models can serve as a basis to support engineering tasks requiring low-fidelity simulation, such as the validation of base control functions during the factory acceptance test.

17/01890 Characterization model for innovative plant designs in the process industry – an application to transformable plants

Wörsdörfer, D. *et al. Chemical Engineering and Processing: Process Intensification*, 2016, 100, 1–18.

This article presents a characterization model for describing, comparing and improving innovative plant designs based on the core idea of quality function deployment. The presented model supports providers of innovative plants to develop highly customer orientated products, to offer a competitive product portfolio and to create customized solutions. Plant operator's requirements are correlated with design attributes. Radar diagrams visualize requirements attainments and indicate individual strengths and weaknesses of the design. In addition the degree of attraction is introduced and specified as a characteristic, comparable performance parameter among innovative plant designs. In order to identify and classify plant operator's requirements a survey in the means of Kano's theory has been conducted. Classified requirements are weighted in order to set up the characterization model. Transformable plant designs are applied in this work as they currently represent a highly discussed example of innovative plants in process industry. As there are several transformable designs in research and practice aiming for different purposes a morphology has been developed in order to be able to define each individual design. Using the morphology for defining design attributes in the model allows a characterization of transformable plants. It is shown that transformable designs lead to highly attractive plants.

17/01891 Characterization of recombination properties at diffused surfaces for industrial silicon solar cell concepts

Rahman, M. M. *et al. Solar Energy*, 2016, 135, 215–221.

This paper describes an experiment to evaluate the surface recombination properties of phosphorous diffused surfaces for crystalline silicon solar cells. In this experiment the analysis of surface recombination properties for the phosphoryl chloride ($POCl_3$) diffusion is carried out. Investigation of recombination properties on diffused surfaces is crucial for the conversion efficiency of silicon solar cells. Hence, the dark saturation current densities (J_o) are determined via quasi steady state photoconductance (QSSPC) decay measurement and the doping profiles by electrochemical-capacitance voltage (ECV) measurement. All the diffusion processes are performed in a quartz tube furnace. The samples are diffused at peak temperatures of 800–950 °C. Therefore; the influence of several parameters for example the extent of surface concentration, the diffusion temperature and the dark saturation current density (J_o) are evaluated.

17/01892 CPFD modeling and experimental validation of gas–solid flow in a down flow reactor

Lanza, A. *et al. Computers & Chemical Engineering*, 2016, 90, 79–93.

This paper reports the fluid dynamics in the developed flow region of a cocurrent gas–solid down flow fluidized bed unit. Gas–solid flows are simulated using a computational particle fluid dynamics (CPFD) numerical scheme and experimental data from the CREC-GS-Optiprobes. This model represents clusters in a downer unit. It is hypothesized that in downers, clusters are formed via a random particle-selection method (RPSM) ensuring cluster dynamic stability. To accomplish this, a statistical particle-selection of clusters (SPSC) method is developed. This hybrid model is validated with experimental data obtained in a 2 m height and 2.57 cm diameter column. Observed time-averaged axial and radial velocities and solid concentration profiles are successfully simulated by the Hybrid CPFD/CREC-GS-Optiprobes data model. These findings support: (a) a narrow distribution of particle cluster residences, (b) the relatively flat radial solid concentrations and solid cluster velocities, and (c) a valuable approach for establishing slip velocities in downer units.

17/01893 Cryogenic flat-panel gas-gap heat switch

Vanapalli, S. *et al. Cryogenics*, 2016, 78, 83–86.

A compact additive manufactured flat-panel gas-gap heat switch operating at cryogenic temperature is reported in this paper. A guarded-hot-plate apparatus has been developed to measure the thermal conductance of the heat switch with the heat sink temperature in the range of 100–180 K. The apparatus is cooled by a two-stage GM cooler and the temperature is controlled with a heater and a braided copper wire connection. A thermal guard is mounted on the hot side of the device to confine the heat flow axially through the sample. A gas handling system allows testing the device with different gas pressures in the heat switch. Experiments are performed at various heat sink temperatures, by varying gas pressure in the gas-gap and with helium, hydrogen and nitrogen gas. The measured off-conductance with a heat sink temperature of 115 K and the hot plate at 120 K is 0.134 W/K, the on-conductance with helium and hydrogen gases at the same temperatures is 4.80 and 4.71 W/K, respectively. This results in an on/off conductance ratio of 37 ± 7 and 35 ± 6 for helium and hydrogen respectively. The experimental results matches fairly well with the predicted heat conductance at cryogenic temperatures.

17/01894 Dynamic simulation of a triple-pressure combined-cycle plant: hot start-up and shutdown

Mertens, N. *et al. Fuel*, 2016, 167, 135–148.

The operation of combined-cycle power plants is increasingly determined by frequent start-ups and shutdowns for grid balancing. This study investigates the capability of a comprehensive process simulation model to predict the transient response of a triple-pressure heat recovery steam generator (HRSG) with reheater to the start-up and shutdown procedures of a heavy-duty gas turbine. The model is based on geometry data, system descriptions and heat transfer calculations established in the original HRSG design. The numerical solution approach and the practical development of a suitable model structure, including the required control circuits, are explained. Detailed simulation results are presented, using initial conditions that correspond to a previous overnight shutdown. Calculations are performed for a complete operating cycle of the plant, where the following main phases are distinguished: start-up procedure, load-following operation, design operation and shutdown procedure. The numerical model is validated with measurement data of the commercial power plant for each pressure stage, yielding good agreement. Deviation from the transient behaviour of the real plant is discussed with regard to modelling assumptions and incomplete information on components outside the HRSG system boundaries.

17/01895 Fischer–Tropsch synthesis product selectivity over an industrial iron-based catalyst: effect of process conditions

Todic, B. *et al. Catalysis Today*, 2016, 261, 28–39.

The effect of process conditions on product selectivity of Fischer–Tropsch synthesis (FTS) over industrial iron-based catalyst (100 Fe/5 Cu/4.2 K/25 SiO_2) was studied in a 1-L stirred tank slurry reactor. Experiments were performed over a range of different reaction conditions, including three temperatures ($T = 493$, 513 and 533 K), four pressures ($P = 0.8$, 1.5, 2.25 and 2.5 MPa), two synthesis gas feed molar ratios ($H_2/CO = 0.67$ and 2) and gas space velocity from 0.52 to 23.5 Ndm^3/g-Fe/h. The effect of process conditions on reaction pathways of FTS and secondary 1-olefin reactions was analysed by comparing product selectivities, chain growth probabilities and ratios of main products (n-paraffin, 1- and 2-olefin). Reduction of methane production and increase of C_{5+} products was achieved by decreasing temperature, inlet H_2/CO ratio and/or increasing pressure. Overall selectivity toward methane and C_{5+} did not show significant changes with variations in residence time. All of the product selectivity variations were shown to be related to changes in chain length dependent growth probabilities.

17/01896 Implementation of a cogeneration plant for a food processing facility. A case study

Bianco, V. *et al. Applied Thermal Engineering*, 2016, 102, 500–512.

This paper presents an investigation regarding the feasibility analysis of a cogeneration plant for a food processing facility with the aim to decrease the cost of energy supply. The monthly electricity and heat consumption profiles are analysed, in order to understand the consumption profiles, as well as the costs of the current furniture of electricity and gas. Then, a detailed thermodynamic model of the cogeneration cycle is implemented and the investment costs are linked to the thermodynamic variables by means of cost functions. The optimal electricity power of the co-generator is determined with reference to various investment indexes. The analysis highlights that the optimal dimension varies according to the chosen indicator, therefore it is not possible to establish it univocally, but it depends on the financial/economic strategy of the company through the considered investment index.

17/01897 Improvement of the energy generation by pressure retarded osmosis

Nagy, E. *et al. Energy*, 2016, 116, 1323–1333.

Applying the solute fluxes given for every single transport layer, namely external boundary layers, selective and the support layer, and even the cake layer, new expressions were developed to define the overall mass transfer coefficient and the interface solute concentrations. These equations make possible much deeper investigation of the mass transport process and process efficiency in pressure retarded osmosis system. It was stated that the effect of the feed side boundary layer on the energy generation must not be neglected without checking its effect. The extractable energy is dominated mainly by the membrane selectivity, structural parameter and also by the solute concentrations.

Essential improvement of the membrane selectivity and/or decrease of the value of the structural parameter is needed to get more efficient pressure retarded osmosis process for energy extraction. Furthermore the increase of the draw solution concentration and/or decrease of the feed concentration should be regarded as an alternative process instead of seawater–river water pair.

17/01898 Jointly optimized control for reverse osmosis desalination process with different types of energy resource

Lee, S. *et al. Energy*, 2016, 117, 116–130.

High-energy efficiency for low operating cost of desalination can be obtained from operational optimizations as well as component-wise innovations. This paper is concerned with an energy-efficient operation for reverse osmosis (RO) desalination process involving a joint control of multiple modules. Energy resource considered for desalination is of two types: intermittent solar energy and steady grid energy. With solar energy, the energy efficiency is measured by total permeate production obtained while the solar energy is available. With grid energy, the energy efficiency is measured by the power consumed to get unit permeate production rate. Achieving maximum energy efficiency is equivalent to solving constrained optimization. For the constrained optimization, obligatory constraints are given by the permissible ranges of trans-membrane pressure on RO membrane and total dissolved solids of permeate, and optional constraint is given by the permissible range of permeate production rate. Constraints as well as the objective function are modelled by the empirical second order equations in terms of control variables of multiple modules. Jointly optimal values of the control variables are found by the sequential quadratic programming. Experimental results obtained by the jointly optimal control demonstrate superior performances as compared to those acquired by marginally optimal control schemes.

17/01899 Numerical investigation on species transport in electroslag remelting dual alloy ingot

Wang, Q. *et al. Applied Thermal Engineering*, 2016, 103, 419–427.

A transient three-dimensional (3D) comprehensive model has been developed to investigate the solute transport in electroslag remelting (ESR) dual alloy ingot. The solutions of the mass, momentum, energy, and species conservation equations were simultaneously calculated by the finite volume method, and full coupling of the Joule heating and Lorentz force through the solving Maxwell's equations. The movement of the metal droplet was described with the volume of fluid (VOF) approach. Besides, the solidification was modelled by using an enthalpy-based technique, where the mushy zone was treated as a porous medium with an anisotropic permeability. A reasonable agreement between the simulation and the experiment was obtained. The results indicate that the colder metal flowing downward washes the solidification front in the process. The solute-poor metal in the pool displaces the solute-rich metal in the mush region. Meanwhile, the solute enrichment promotes the sinking of the liquid. The inward Lorentz force pushes the metal from the periphery to the bottom. The solutes are deposited at the pool bottom. The negative segregation occurs in the lower part and then rises to positive for the two elements. The maximal positive and negative segregation indexes of the carbon and nickel along the vertical centreline of the ESR dual alloy ingot are 0.38 and −0.19, and 0.15 and −0.02, respectively.

17/01900 Optimal design and operation of an industrial three phase reactor for the oxidation of phenol

Mohammed, A. E. *et al. Computers & Chemical Engineering*, 2016, 94, 257–271.

Among several treatment methods catalytic wet air oxidation (CWAO) treatment is considered as a useful and powerful method for removing phenol from waste waters. In this work, mathematical model of a trickle bed reactor (TBR) undergoing CWAO of phenol is developed and the best kinetic parameters of the relevant reaction are estimated based on experimental data (from the literature) using parameter estimation technique. The validated model is then utilized for further simulation and optimization of the process. Finally, the TBR is scaled up to predict the behaviour of CWAO of phenol in industrial reactors. The optimal operating conditions based on maximum conversion and minimum cost in addition to the optimal distribution of the catalyst bed is considered in scaling up and the optimal ratio of the reactor length to reactor diameter is calculated with taking into account the hydrodynamic factors (radial and axial concentration and temperature distribution).

17/01901 Quick assessment of binary distillation efficiency using a heat engine perspective

Blahušiak, M. *et al. Energy*, 2016, 116, 20–31.

With emphasis on close boiling (near-)ideal vapour–liquid equilibrium mixtures, this paper links the efficiency of distillation to the binary feed composition and thermal properties of the compounds. The proposed approach, treating the process as a heat engine, allows to directly quantify distillation performance (in terms of energy intensity & efficiency) based on the components boiling points and feed composition. In addition, this approach reviews and formulates simple, approximate and essentially non-iterative calculation procedures to quickly estimate the energy efficiency of distillation. These estimations may be applied to identify opportunities to save significant amounts of energy. The results show that the reboiler duty for low relative volatility is relatively independent of the heat of vaporization and feed composition, while being reciprocally proportional to the Carnot efficiency of the distillation column. The internal efficiency for distillation of mixtures with low relative volatility has a maximum of about 70% for a symmetrical feed (equimolar ratio) and decreases to zero for unsymmetrical feed compositions approaching infinite dilution. With increasing relative volatility, the maximum efficiency is preserved, but the locus shifts towards lower light component fractions. At very high relative volatility, the internal efficiency increases with decreasing concentration of light component, as typical for evaporators.

17/01902 Retrofit of low-temperature heat recovery industrial systems using multiobjective exergoeconomic optimization

Deslauriers, M.-A. *et al. Energy Conversion and Management*, 2016, 130, 207–218.

Reducing the energy consumption of a plant often conflicts with the investment required for heat recovery. This paper presents a design study of shell and tube heat exchanger and direct-contact heat exchanger in three retrofit configurations. Multiobjective optimizations are employed to find optimal solutions that increase exergy efficiency at justifiable costs. A numerical modelization of heat transfer equipment is developed using heat transfer, pressure drop and cost correlations from the open literature. In order to verify the capability of the proposed approach, a case study for heat recovery in a pulp and paper plant is presented. In which multiple structural modifications of existing heat recovery systems are proposed based on an analysis of the Grand Composite Curve pinch targeting method. Each proposed modification is subject to multiobjective optimization based on the fast non-dominant sorting genetic algorithm (NSGA-II). The case study's results shows significant steam operation cost reduction of up to 89% reducing exergy destruction by 82%. It has also been shown that for some heat recovery modifications the most cost effective solution is close to the minimum exergy destruction solution subject to equipment design constraints.

17/01903 Strategy-making for a proactive distribution company in the real-time market with demand response

Zhang, C. *et al. Applied Energy*, 2016, 181, 540–548.

This paper proposes a methodology to optimize the trading strategies of a proactive distribution company (PDISCO) in the real-time market by mobilizing the demand response. Each distribution-level demand is considered as an elastic one. To capture the interrelation between the PDISCO and the real-time market, a bi-level model is presented for the PDISCO to render continuous offers and bids strategically. The upper-level problem expresses the PDISCO's profit maximization, while the lower-level problem minimizes the operation cost of the transmission-level real-time market. To solve the proposed model, a primal-dual approach is used to translate this bi-level model into a single-level mathematical program with equilibrium constraints. Results of case studies are reported to show the effectiveness of the proposed model.

17/01904 Teaching an old dog new tricks: firm learning from environmental regulation

Galloway, E. and Johnson, E. P. *Energy Economics*, 2016, 59, 1–10.

This study examines a new mechanism by which environmental regulation can increase efficiency: intra-firm knowledge spillovers due to environmental regulation. County-level non-attainment of the National Ambient Air Quality Standards creates spatial variation in the degree of regulatory stringency, as states impose stronger environmental regulation in non-attainment counties. This spatial variation is used to examine how the efficiency of electricity generators responds to increases in regulation. It is shown that, in response to increased regulatory stringency, electricity generators find technical efficiency enhancements and then transfer these enhancements to other units within their fleet. The authors found that a change in regulatory stringency translates to within-firm spillovers of 3–4%, and that these gains occur at least 3 years after the increase in regulatory stringency.

10 SPACE HEATING AND COOLING/HEAT PUMPS

17/01905 A compact cryogenic pump

Li, G. *et al. Cryogenics*, 2016, 75, 35–37.

A centrifugal cryogenic pump has been designed at Argonne National Laboratory to circulate liquid nitrogen (LN_2) in a closed circuit allowing the recovery of excess fluid. The pump can circulate LN_2 at rates of 2–10 L/min, into a head of 0.5–3 m. Over 4 years of laboratory use the pump has proven capable of operating continuously for 50–100 days without maintenance.

17/01906 A model for the performance assessment of hybrid coolers by means of transient numerical simulation

D'Antoni, M. *et al. Applied Energy*, 2016, 181, 477–494.

This paper presents the development of a numerical model of a hybrid cooler for transient simulation purposes as a component of a thermal energy system. The model uses a modular definition of the control volume, and is suitable for modelling any staggered coil geometry. The set of parameters required for modelling the hybrid cooler is typical of the so-called design models. A rigorous analysis of sensible and latent heat fluxes due to spray water evaporation is included. Further, the model can be exploited for the development of user-defined control strategies of fans and water spray systems. The model is validated using monitored data from a pilot system installation in which a commercial hybrid cooler is operated under typical summer south European working conditions.

17/01907 Adoption of enclosure and windbreaks to prevent the degradation of the cooling performance for a natural draft dry cooling tower under crosswind conditions

Wang, W. *et al. Energy*, 2016, 116, 1360–1369.

Crosswind degrades the cooling performance of a natural draft dry cooling tower (NDDCT) by affecting the air flow field at the inlet and outlet and inducing complex vortices inside and outside the tower. The distribution of the vortices along the flow streams is found to be a key factor for the ventilation rate. The parameter of flow loss factor is proposed to quantitatively identify the effect of the vortices and unbalanced flow on the ventilation rate. Approaches of the installations of windbreaks and enclosure on the cooling performance of the NDDCT are numerically studied. It is found that both approaches can individually reduce the size of the inner wall vortex, improving the flow field characteristics. However, they have different strengths in breaking up the side low pressure areas and reducing the swirling intensity of the mainstream vortices. Results show that the approaches of windbreaks and enclosure can effectively prevent the degradation of the cooling performance for the NDDCT in a wide crosswind velocity range, and their combination could nearly eliminates the negative effect of the crosswind.

17/01908 Amplified charge and discharge rates in phase change materials for energy storage using spatially-enhanced thermal conductivity

Wei, L. C. and Malen, J. A. *Applied Energy*, 2016, 181, 224–231.

Composites made with high thermal conductivity meshes embedded in phase change materials (PCMs) increase charge/discharge rates of latent heat energy storage systems. Here the authors consider the benefits of spatially dependent enhancements to thermal conductivity on the charge/discharge rates of PCMs in both one-dimensional Cartesian and one-dimensional cylindrical coordinates. The non-dimensionalized quasi-steady (Stefan number $\lesssim 0.1$) solution indicates that the average charge (discharge) rate in a spatially enhanced PCM outperforms the uniformly enhanced case by maximizing the enhancement near the heat source and therein reducing the time averaged thermal resistance to melting (solidifying). Relative to a uniformly enhanced thermal conductivity, the optimal charge/discharge rate enhancement is a modest 12% in one-dimensional Cartesian coordinates but as high as 140% in one-dimensional cylindrical coordinates. These analytical solutions are a design guide for graded mesh structures that can be realized by advanced fabrication techniques such as additive manufacturing and applied in applications ranging from telecommunications to buildings, where PCMs are employed to harness rapidly varying energy sources.

17/01909 An explanation of the Al_2O_3 nanofluid thermal conductivity based on the phonon theory of liquid

Iacobazzi, F. *et al. Energy*, 2016, 116, 786–794.

In the present work a systematic investigation on several mechanisms affecting the thermal conductivity of alumina-based nanofluid, such as layering, Brownian motion, clustering, ballistic phonon motion, thermal boundary resistance and mass difference scattering, is presented. The effect of mass difference scattering is for the first time suggested and studied in the present work. Both theoretical and experimental approaches have been carried out in order to analyse the competition of these phenomena and to identify the most relevant. This was obtained by comparing micrometric and nanometric particles suspended in liquid water (293 K), frozen water (253 K) and diathermic oil (293 K). Each of the above-mentioned conditions was selected to make dominant only one of the mechanisms that affect nanofluid thermal conductivity. The main results of this investigation concern the mass difference scattering, which has been found to be the most intensive mechanism reducing the nanofluid thermal conductivity with respect to the microfluid one.

17/01910 An inquiry into the reliability of window operation models in building performance simulation

Tahmasebi, F. and Mahdavi, A. *Building and Environment*, 2016, 105, 343–357.

Given the impact of inhabitants' control actions on indoor environment and the complex nature of such interactions, sophisticated models of occupants' presence and behaviour are increasingly deployed to enhance the reliability of building performance simulations. However, the use of occupant behaviour models in building simulation efforts and their predictive performance in different contexts involves potentially detrimental uncertainties. To address this issue, the present study deploys long-term monitored data from an office area and its calibrated simulation model to conduct an external evaluation of a number of stochastic and non-stochastic window operation models in view of their (a) potential in predicting occupants' operation of windows, and (b) effectiveness to enhance the reliability of building performance simulation efforts. The results suggest that, while stochastic models can emulate the seemingly random character of occupant behaviour and provide probabilistic distributions of performance indicators, their use does not guarantee more reliable predictions. Leaving aside the large errors resulted from using such models without the necessary adjustments, stochastic window operation models overestimated the occupants' operation of windows in heating season and thus the annual and peak heating demands. However, as compared with rule-based models, the stochastic models displayed a better performance in predicting window operations and thermal comfort assessment in the free-running season.

17/01911 Automated heat exchanger network synthesis by using hybrid natural algorithms and parallel processing

Pavão, L. V. *et al. Computers & Chemical Engineering*, 2016, 94, 370–386.

Heat exchanger network (HEN) synthesis can be formulated as an optimization problem, which can be solved by meta-heuristics. These approaches account for a large computational time until convergence. In the present paper the potentialities of applying parallel processing techniques to a non-deterministic approach based on a hybridization between genetic algorithms (GA) and particle swarm optimization (PSO) were investigated. Six literature examples were used as benchmarks for the solutions obtained. Comparative experiments were carried out to investigate the time efficiency of the method while implemented using series or parallel processing. The solutions obtained led to lower total annual costs than those presented by the literature. As expected, parallel processing usage multiplied the algorithm speed by the number of cores used. Hence, it can be concluded that the proposed method is capable of finding excellent local optimal solutions, and the application of multiprocessing techniques represented a substantial reduction in execution time.

17/01912 Can radiant floor heating systems be used in removable glazed enclosed patios meeting thermal comfort standards?

Garcia, D. A. *Building and Environment*, 2016, 106, 378–388.

Many systems are used for heating glazed enclosed patios of restaurants, pubs or other restaurant businesses. This paper explores the possibilities of use radiant floor heating systems (RFHS) in removable glazed enclosed patios maintaining thermal comfort in terms of predicted percentage of dissatisfied (PPD) and predicted mean vote (PMV) optimal ranges. The effects of different envelope structures of glazed enclosed patios on floor surface temperature using a radiant floor heating system have been analysed. In addition, considering the use of removable and modular radiant floor heating panels, delivery and return pipes layouts from a heat power generator to each single radiant floor heating panel have been analysed assessing flow velocity and pressure drops in order to pinpoint the best layout for optimizing heat transfer efficiency and energy saving. The findings showed at assumed outdoor and indoor temperatures what are the considered glazed enclosed patio envelopes that allow the use of a RFHS maintaining the floor surface temperature within thermal comfort ranges and avoiding local thermal discomfort due to floor temperature and vertical radiation asymmetry. Moreover, the flow velocity and concentrated/distributed pressure drops analysis pinpointed optimal pipe layouts for connecting heat power generator to

each underfloor heating panel. concluding, the paper highlighted that, up to meet thermal comfort standards, under floor heating systems could be used for heating glazed enclosed patios only for certain envelope structures. Additionally, a delivery and return pipe layout should be properly designed for minimizing pressure drops and optimize heat transfer efficiency.

17/01913 Cellulose/graphene aerogel supported phase change composites with high thermal conductivity and good shape stability for thermal energy storage

Yang, J. *et al. Carbon*, 2016, 98, 50–57.

As phase change composites, high thermal conductivity, large latent heat of fusion and good shape stability are all required for practical applications. By combining defect-free graphene nanoplatelets (GNPs) and microcrystalline cellulose, lightweight cellulose/GNP aerogels are fabricated and their highly porous but strong three-dimensional networks benefit the encapsulation of polyethylene glycol (PEG) and prevent the leakage of PEG above its melting point. Phase change composites are prepared by vacuum-assisted impregnating of PEG into the cellulose/GNP aerogels, which exhibit high thermal conductivity, good shape stability and high latent heat of fusion. Even compressed upon the melting point of PEG, the phase change composites keep their shapes stable without any leakage. With only 5.3 wt% of GNPs, the composite exhibits a high thermal conductivity of 1.35 $W m^{-1} K^{-1}$, 463% higher than that of the composite without GNPs. The highly porous cellulose network and the low loading of highly thermally conductive GNPs are responsible for the high loading of PEG in the composite with a satisfactory latent heat of fusion of 156.1 $J g^{-1}$.

17/01914 CFD aided approach to design printed circuit heat exchangers for supercritical CO_2 Brayton cycle application

Kim, S. G. *et al. Annals of Nuclear Energy*, 2016, 92, 175–185.

While most conventional printed circuit heat exchangers (PCHE) designs for working fluid of supercritical CO_2 require an extension of valid Reynolds number limits of experimentally obtained correlations, computational fluid dynamics (CFD) code ANSYS CFX was used to explore validity of existing correlations beyond their tested Reynolds number ranges. For heat transfer coefficient correlations, an appropriate piece-wising with Ishizuka's and Hesselgreaves's correlation is found to enable an extension of Reynolds numbers. For friction factors, no single existing correlation is found to capture different temperature and angular dependencies for a wide Reynolds number range. Based on the comparison of CFD results with the experimentally obtained correlations, a new CFD-aided correlation covering an extended range of Reynolds number 2000–58,000 for Nusselt number and friction factor is proposed to facilitate PCHE designs for the supercritical CO_2 Brayton cycle application.

17/01915 CFD analysis of a diaphragm free-piston Stirling cryocooler

Caughley, A. *et al. Cryogenics*, 2016, 79, 7–16.

This paper presents a computational fluid dynamics (CFD) analysis of a novel free-piston Stirling cryocooler that uses a pair of metal diaphragms to seal and suspend the displacer. The diaphragms allow the displacer to move without rubbing or moving seals. When coupled to a metal diaphragm pressure wave generator, the system produces a complete Stirling cryocooler with no rubbing parts in the working gas space. Initial modelling of this concept using the Sage modelling tool indicated the potential for a useful cryocooler. A proof-of-concept prototype was constructed and achieved cryogenic temperatures. A second prototype was designed and constructed using the experience gained from the first. The prototype produced 29 W of cooling at 77 K and reached a no-load temperature of 56 K. The diaphragm's large diameter and short stroke produces a significant radial component to the oscillating flow fields inside the cryocooler which were not modelled in the one-dimensional analysis tool Sage that was used to design the prototypes. Compared with standard pistons, the diaphragm geometry increases the gas-to-wall heat transfer due to the higher velocities and smaller hydraulic diameters. A CFD model of the cryocooler was constructed to understand the underlying fluid-dynamics and heat transfer mechanisms with the aim of further improving performance. The CFD modelling of the heat transfer in the radial flow fields created by the diaphragms shows the possibility of utilizing the flat geometry for heat transfer, reducing the need for, and the size of, expensive heat exchangers. This paper presents details of a CFD analysis used to model the flow and gas-to-wall heat transfer inside the second prototype cryocooler, including experimental validation of the CFD to produce a robust analysis.

17/01916 Characterization of granular phase change materials for thermal energy storage applications in fluidized beds

Izquierdo-Barrientos, M. A. *et al. Applied Energy*, 2016, 181, 310–321.

This work investigates commercially available granular phase change materials (PCMs) with different transition temperatures for the use of thermal-energy storage systems in fluidized beds. The hydrodynamic characteristics of granular PCMs were tested in cylindrical-3D and planar-2D fluidized beds. The density, particle size distribution and angle of repose were measured for various PCM materials. Further attrition studies were conducted with changes in particle surface from abrasion, which were characterized using a scanning electron microscope. The results indicate that some materials with smaller particle size and thinner supporting structure can lose the paraffin during the fluidization process, when paraffin is in a liquid state. As a consequence, the particles agglomerate, and the bed defluidizes. For all of the tested materials, only GR50 (with a transition temperature of 50 °C) properly fluidizes when the paraffin is in the liquid state and has shown to endure >75 h of continuous operation and 15 melting-solidification cycles in a fluidized bed. Additional differential scanning calorimetry measurements of the cycled particles did not show a decrease in energy storage capacity of the granular PCM, which corroborates that there is no loss of material after >75 h of fluidization.

17/01917 Comparison of solar dryer and solar-assisted heat pump dryer for cassava

Yahya, M. *et al. Solar Energy*, 2016, 136, 606–613.

The performance of a solar dryer (SD) and a solar-assisted heat pump dryer (SAHPD) for drying of cassava chips have been investigated. The SD and SAHPD decreased the mass of cassava from 30.8 to 17.4 kg within 13 and 9 h at average temperatures of 40 and 45 °C, respectively. The moisture content of cassava decreased from 61% (wet basis) to 10.5%, with a mass flow rate of 0.124 kg/s. The average thermal efficiencies were 25.6% and 30.9% for SD and SAHPD, respectively. The average drying rate (DR) and specific moisture extraction rate (SMER) were 1.33 kg/h and 0.38 kg/kW h, respectively, for SD as well as 1.93 kg/h and 0.47 kg/kW h, respectively, for SAHPD. The pick-up efficiencies varied from 3.9% to 65.8% and 15.9% to 70.4% for SD and SAHPD, with average values of 39.3% and 43.6%, respectively. The average solar fractions were 66.7% for SD and 44.6% for SAHPD. The coefficient of performance of the heat pump ranged from 3.23 to 3.47, with an average of 3.38.

17/01918 Correct integration of compressors and expanders in above ambient heat exchanger networks

Fu, C. and Gundersen, T. *Energy*, 2016, 116, 1282–1293.

The appropriate placement concept (also referred to as correct integration) is fundamental in pinch analysis. The placement of reactors, distillation columns, evaporators, heat pumps and heat engines in heat exchanger networks is well established. The placement of pressure changing equipment such as compressors and expanders is complex and less discussed in literature. A major difficulty is that both heat and work (not only heat) are involved. The integration of compressors and expanders separately into heat exchanger networks was recently investigated. A set of theorems were proposed for assisting the design. The problem is even more complex when both compressors and expanders are to be integrated. An important concern is about the sequence of integration with compressors and expanders, i.e. should compressors or expanders be implemented first. This problem is studied and a new theorem is formulated related to the correct integration of both compressors and expanders in above ambient heat exchanger networks. The objective is to minimize exergy consumption for the integrated processes. A graphical design methodology is developed for the integration of compressors and expanders into heat exchanger networks above ambient temperature.

17/01919 Daily cooling of one-story buildings using domed roof and solar adsorption cooling system

Poshtiri, A. H. *et al. Applied Energy*, 2016, 182, 299–319.

This study investigates a new system which utilizes a solar-driven adsorption chiller to provide natural cooling of a one-storey building with domed roof, theoretically. The domed roof provides natural ventilation, and the ambient air flowing into the building is cooled in a cooling channel with the assistance of the adsorption chiller. The influence of geometric parameters such as the size of the inlet and outlet vent, and the depth of the cooling channel on air change per hour (ACH) is studied. In addition, the room temperature is evaluated for different values of room cooling demand and ACH, under different ambient conditions. The system's ability to provide thermal comfort in the room is also investigated. The results show that ACH can be controlled by changing the size of the inlet air vent. It is also found that adaptive thermal comfort condition (ATCS) is achieved under larger cooling demand values when ACH goes up. Furthermore, use of three cooling plates in the channel instead of two plates increases the maximum cooling demand for which thermal comfort is achieved, according to ATCS, from 775 to 1295 W. Moreover, application of the proposed system for cooling of a building in Bandar Abbas consumes 45% less electric energy in comparison with a split air conditioner of the same capacity.

17/01920 Designing and optimizing a novel advanced adiabatic compressed air energy storage and air source heat pump based μ-combined cooling, heating and power system

Jabari, F. *et al. Energy*, 2016, 116, 64–77.

This paper presents the design and optimum scheduling of a solar combined cool, heat and power system which is powered by a Stirling engine in the presence of an advanced adiabatic compressed air energy storage (AA-CAES) system for a residential energy sector. An absorber and a thermal energy storage tank are employed to absorb and store all collected solar radiation for continuous energy supplied when sunlight is insufficient, and night-time. In this paper, an air source heat pump (ASHP) that is equipped with two inside and outside air fans, an expansion valve, compressor, condenser and an evaporator is installed to cool and heat a benchmark residential building under hot and cold climate conditions, respectively. The AA-CAES system is modelled with injected and produced power constraints, storage, air balance and operation limits. A comprehensive energy and exergy based optimization is developed as a mixed-integer non-linear program to minimize total energy procurement cost in the presence of ASHP, prime mover and AA-CAES's constraints. It is found that the use of AA-CAES results in 21.79% and 22.36% lower operational costs in the cooling and the heating modes, respectively.

17/01921 Development of an exergoeconomic model for analysis and multi-objective optimization of a thermoelectric heat pump

Nemati, A. *et al. Energy Conversion and Management*, 2016, 130, 1–13.

A thermoelectric heat pump (TEHP) is modelled, analysed and optimized from the viewpoint of energy, exergy and exergoeconomic. A comprehensive parametric study is also done to clarify the effects on the energy, exergy and exergoeconomic performance of some main decision parameters. With the aim of exergetic and economic optimization, an optimization methodology based on multi-objective genetic algorithm is applied to the system and optimal values of design variables are obtained. Two objective functions are considered; exergy efficiency and unit cost of heating power. It is observed that the performance of TEHP is comparable to conventional heat pumps from the viewpoints of thermodynamic and exergoeconomic. SPECO method is applied to evaluate the exergoeconomic parameters. The results demonstrate that all decision parameters except the number of thermocouples optimize exergy efficiency and coefficient of performance of the TEHP. The obtained overall exergoeconomic factor of 60.6% illustrates that the 39.4% of total system cost relates to exergy destruction. Under optimal conditions, the unit cost of heating power and exergy efficiency are found to be 0.688 $/kW h and 14.13%, respectively.

17/01922 Development of micro-scale axial and radial turbines for low-temperature heat source driven organic Rankine cycle

Al Jubori, A. *et al. Energy Conversion and Management*, 2016, 130, 141–155.

Most studies on the organic Rankine cycle (ORC) focused on parametric studies and selection working fluids to maximize the performance of organic Rankine cycle but without attention for turbine design features which are crucial to achieving them. The rotational speed, expansion ratio, mass flow rate and turbine size have markedly effect on turbine performance. For this purpose ORC modelling, mean-line design and three-dimensional computational fluid dynamics analysis were integrated for both micro axial and radial-inflow turbines with five organic fluids (R141b, R1234yf, R245fa, *n*-butane and *n*-pentane) for realistic low-temperature heat source $<100\,^{\circ}C$ like solar and geothermal energy. Three-dimensional simulation is performed using ANSYS^{R17}-CFX where three-dimensional Reynolds-averaged Navier–Stokes equations are solved with k-omega shear stress transport turbulence model. Both configurations of turbines are designed at wide range of mass flow rate (0.1–0.5) kg/s for each working fluid. The results showed that *n*-pentane has the highest performance at all design conditions where the maximum total-to-total efficiency and power output of radial-inflow turbine are 83.85% and 8.893 kW, respectively. The performance of the axial turbine was 83.48% total-to-total efficiency and 8.507 kW power output. The maximum overall size of axial turbine was 64.685 mm compared with 70.97 mm for radial-inflow turbine. R245fa has the lowest overall size for all cases. The ORC thermal efficiency was about 10.60% with radial-inflow turbine and 10.14% with axial turbine. Such results are better than other studies in the literature and highlight the potential of the integrated approach for accurate prediction of the ORC performance based on micro-scale axial and radial-inflow turbines.

17/01923 Diurnal performance analysis of phase change material walls

Kara, Y. A. *Applied Thermal Engineering*, 2016, 102, 1–8.

A research study was conducted to investigate the thermal performance of phase change material (PCM) walls. The south-facing external wall of a test room was constructed using PCM walls composed of brick walls, plasterboards containing PCMs, and novel triple glass. The thermal performance of the PCM walls was experimentally determined on a daily basis. The ratio of the solar energy gain provided by the PCM walls to the heat load of the test room on a daily basis varied from 12% to 25%; daily overall efficiency of the coupled novel triple glass and PCM walls varied from 17% to 20%; and solar transmittance of the novel triple glass varied from 45% to 55% during the heating period.

17/01924 Effect of installation angle of fins on melting characteristics of annular unit for latent heat thermal energy storage

Yuan, Y. *et al. Solar Energy*, 2016, 136, 365–378.

Latent heat thermal energy storage (LHTES) technology can solve the problem of a mismatch between energy supply and demand in time, space and intensity and thus has become a research on focus in energy and environmental protection. The low thermal conductivity of phase change materials (PCMs) is the primary bottleneck of the popularization application of LHTES technology. An effective way to solve this problem is adding fins into the PCM container to enhance heat transfer, there has been no report on the effect of the installation location of fins on the heat transfer characteristics of the PCM in a LHTES unit. To study the effect of fins installed at different locations on the heat transfer, this work have investigated the melting characteristics of PCM in an annular with different installation angle of fins (θ) via a numerical simulation method, which is based on an enthalpy-porous medium model. In addition, the numerical calculation results are verified via experimentation. On this basis, the melting processes of the PCM in horizontal, annular units with fins installed at five different values of θ under three fixed wall temperature conditions (60, 70 and 80 °C) have been simulated. The simulation results have been compared to those of the unit without fins. The results show that although fins inhibit natural convection, the addition of fins can lead to an increase in the melting rate and a decrease in the melting time due to an increase in the total amount of heat exchanged. Considering the entire melting process, the melting rate of the PCM in the unit with fins installed at $\theta = 0^{\circ}$ is maximum. When θ reaches 45°, the further increase of θ has no marked impact on the melting rate of the PCM in the unit. Based on the trend of the change of the mean Nusselt number with the Fourier number (*Fo*), the heat transfer of the melting process of the PCM is divided into four stages. Additionally, the dimensionless criterion relationship between the melting fraction (f) and $SteFoRa^{1/6}$ when $\theta = 0^{\circ}$ is fitted as $f = 0.24X^3 - 1.13X^2 + 1.82X$, where $X = SteFoRa^{1/6}$.

17/01925 Encapsulation of phase change materials using rice-husk-char

Gondora, W. *et al. Applied Energy*, 2016, 182, 274–281.

This paper explored a new approach to prepare phase change microcapsules using carbon-based particles via Pickering emulsions for energy storage applications. Rice-husk-char, a by-product in biofuel production, containing 53.58 wt% of carbon was used as a model carbon-based material to encapsulate hexadecane. As a model phase change material, hexadecane was emulsified in aqueous suspensions of rice-husk-char nanoparticles. Water soluble polymers poly(diallyldimethyl-ammonium chloride) and poly(sodium styrene sulfonate) were used to fix the rice-husk-char nanoparticles on the emulsion droplets through layer-by-layer assembly to enhance the structural stability of the microcapsules. The microcapsules formed are composed of a thin shell encompassing a large core consisting of hexadecane. Thermal gravimetrical and differential scanning calorimeter analyses showed the phase change enthalpy of 80.9 kJ kg^{-1} or 120.0 MJ m^{-3}. Design criteria of phase change microcapsules and preparation considerations were discussed in terms of desired applications. This work demonstrated possible utilizations of biomass-originated carbon-based material for thermal energy recovery and storage applications, which can be a new route of carbon capture and utilization.

17/01926 Evaluation of passive ventilation provision in domestic housing retrofit

Kinnane, O. *et al. Building and Environment*, 2016, 106, 205–218.

Increasing energy efficiency in the residential sector, while maintaining adequate home ventilation for health and well-being, is proving to be a challenge. This study assesses the efficacy of passive ventilation strategies designed to comply with building regulations and imposed after housing energy-efficiency retrofits. In particular, it focuses on the provision of ventilation using background through-wall vents, which remains a common strategy in a number of European countries including Ireland and the UK, where vent sizes, related to floor area, are stipulated in building regulations. A collective of social housing, with background through-wall vents installed post thermal retrofit, is taken as a case study. These homes are modelled to interrogate the impact of the passive ventilation strategy on house air exchange rate

and thermal heating energy loads. The reaction of occupants to through-wall vent installation is decidedly negative and many block vents to limit thermal discomfort and heat loss. Simulation studies show significant external air ingress through vents. A wide range of effective air change rates are observed when vents are sized without reference to building airtightness, and significant energy penalties result for the leakier homes. This study evaluates the provision of passive through-wall ventilation as part of a retrofit programme and shows it to have a number of drawbacks that may impact on the health of the building and its occupants and ultimately be at odds with the aims of achieving energy efficiency in the residential sector.

17/01927 Experiment study on the thermal properties of paraffin/kaolin thermal energy storage form-stable phase change materials

Lv, P. *et al. Applied Energy*, 2016, 182, 475–487.

In this paper, different particle sizes of kaolin were employed to incorporate paraffin via vacuum impregnation method. The paraffin/kaolin composites were characterized by scanning electron microscope, X-ray diffraction, Fourier transform infrared spectroscopy, differential scanning calorimeter and thermogravimetry. The results showed that the paraffin/kaolin composite with the largest particle size of kaolin (K4) has the highest thermal conductivity (0.413 W/(m K) at 20 °C) among the diverse composites. The latent heat capacity of paraffin/K4 is 119.49 J/g and the phase change temperature is 62.4 °C. In addition, the thermal properties and thermal conductivities of paraffin/K4 with different mass fraction of K4 (0–60%) were investigated. The thermal conductivities of the composites were explained in microcosmic field. The phonon mean free path determines the thermal conductivity, and it can be significantly affected by temperature and the contact surface area. The leaks, thermal storage and release properties of pure paraffin and paraffin/kaolin composites were investigated and the composites presented good thermal stabilities.

17/01928 Experimental investigation of the dynamic behavior of a large-scale refrigeration – PCM energy storage system. Validation of a complete model

Wu, J. *et al. Energy*, 2016, 116, 32–42.

In the area of building refrigeration, the use of thermal energy storages coupled with heat pumps is a significant way for reducing the operating costs and optimizing the design of equipment. In this paper, a prototype of large-scale refrigeration – phase change material (PCM) energy storage system is described, from which experimental results on transient behaviour are obtained. A dynamic model for transient simulation of the coupled system is presented. The fluid flows through the heat exchangers and the storage tank are represented by a cascade of continuous stirred tank reactors. Switching procedures between different model configurations associated to phase transitions within heat exchangers and PCM storage tank are mathematically performed by matrix operations. The compressor, the expansion valve and the pressure drop across the evaporator are represented by static models based on empirical correlations. A PI controller for the expansion valve opening is integrated in the heat pump model to maintain the superheat at evaporator exit. The model is validated by a complete and detailed comparison between simulation and experimental results.

17/01929 Experimental study of the influence of cold heat exchanger geometry on the performance of a co-axial pulse tube cooler

Pang, X. *et al. Cryogenics*, 2016, 78, 78–82.

Improving the performance of the pulse tube cooler is one of the important objectives of the current studies. Besides the phase shifters and regenerators, heat exchangers also play an important role in determining the system efficiency and cooling capacity. A series of experiments on a 10 W @ 77 K class co-axial type pulse tube cooler with different cold heat exchanger geometries are presented in this paper. The cold heat exchangers are made from a copper block with radial slots, cut through using electrical discharge machining. Different slot widths varying from 0.12 to 0.4 mm and different slot numbers varying from around 20–60 are investigated, while the length of cold heat exchangers are kept the same. The cold heat exchanger geometry is classified into three groups, namely, constant heat transfer area, constant porosity and constant slot width. The study reveals that a large channel width of 0.4 mm (about 10 times the thermal penetration depth of helium gas at 77 K, 100 Hz and 3.5 MPa) shows poor performance, the other results show complicated interaction effects between slot width and slot number. These systematic comparison experiments provide a useful reference for selecting a cold heat exchanger geometry in a practical cooler.

17/01930 Influence of the pressure-dependent contact area between electrode and composite surface on the electrical conductivity

Liu, X. and Schubert, D. W. *Composite Structures*, 2016, 136, 414–418.

In this work, the influence of the pressure-dependent contact area between electrodes and surfaces of the composite samples on the electrical conductivity of polymer/carbon black composites was investigated. It was found that the electrical conductivity depended on the pressure (P) applied by the testing device and the carbon black concentration (ϕ). Meanwhile, the logarithm of electrical conductivity exhibited a linear relationship with $\phi^{-1/3}$ regardless of the pressures. Furthermore, it was found that the electrical conductivity σ showed a specific relationship ($\log\sigma(P) = kP^{-1} + \log b$) in the pressure range investigated regardless of the concentration. Based on this correlation, the maximum (true) electrical conductivity of the composite samples at a given concentration for infinite pressure can be revealed by extrapolation. Thus, a novel approach is given to eliminate strong variations in electrical conductivity measurements on composites due to imperfect contacts.

17/01931 Investigation of a double oscillating-fan cooling device using electromagnetic force

Su, H.-C. and Xu, H. Y. *Applied Thermal Engineering*, 2016, 103, 553–563.

This study proposes a double oscillating-fan cooling device using electromagnetic force. The device consists of two oscillating-fans. It requires only one electromagnet and two fan sheets with one magnet on each of them. The electromagnet and fan sheets are situated on a base and arranged accordingly. The electromagnetic force generated by the electromagnet can actuate the fan sheets. The main advantage of the device is its simple structure because there is no bearing and motor in the device. The driving current can be either DC PWM (pulse width modulation) or AC (alternating current) within 3–12 V so it is compatible with most electronic devices. The dimensions of the proposed model are 50 mm × 50 mm × 15 mm during operation. Concerning flow rate, sound pressure, power consumption and resonant frequency tests, a comparison between the proposed model and different type of cooling devices has been completed. The result shows that the model can provide cooling ability similar to a rotary fan while consuming 40% of the power of the rotary fan. It shows not only a good cooling ability but also a great potential for structural reliability and design flexibility.

17/01932 Model based approach to synthesize spare-supported cleaning schedules for existing heat exchanger networks

Cheng, K.-Y. and Chang, C.-T. *Computers & Chemical Engineering*, 2016, 93, 413–427.

Almost every modern chemical process is equipped with a heat-exchanger network (HEN) for optimal energy recovery. However, as time goes on after start-up, fouling on the heat-transfer surface in an industrial environment is unavoidable. If the heat exchangers in an operating plant are not cleaned regularly, the targeted thermal efficiency of HEN can only be sustained for a short period of time. To address this practical issue, several mathematical programming models have already been developed to synthesize online cleaning schedules. Although the total utility cost of a HEN could be effectively reduced accordingly, any defouling operation still results in unnecessary energy loss due to the obvious need to temporarily take the unit to be cleaned out of service. The objective of the present study is thus to modify the available model so as to appropriately assign spares to replace them. Specifically, two binary variables are adopted to respectively represent distinct decisions concerning each online exchanger in a particular time interval, i.e. whether it should be cleaned and, if so, whether it should be substituted with a spare. The optimal solution thus includes not only the cleaning schedule but also the total number of spares, their capacities and the substitution schedule. Finally, the optimization results of a series of case studies are also presented to verify the feasibility of the proposed approach.

17/01933 Model-based energy monitoring and diagnosis of telecommunication cooling systems

Sorrentino, M. *et al. Energy*, 2016, 116, 761–772.

A methodology is proposed for on-line monitoring of cooling load supplied by telecommunication (TLC) cooling systems. A sensible cooling load is estimated via a proportional integral controller-based input estimator, whereas a lumped parameters model was developed aiming at estimating air handling units (AHUs) latent heat load removal. The joint deployment of above estimators enables accurate prediction of total cooling load, as well as of related AHUs and free-coolers energy performance. The procedure was then proven effective when extended to cooling systems having a centralized chiller, through model-based estimation of a key performance metric, such as the energy efficiency ratio. The results and experimental validation presented throughout the paper confirm the suitability of the proposed procedure as a reliable and effective energy monitoring and diagnostic tool for TLC applications. Moreover, the proposed modelling approach, beyond its direct contribution towards smart use and

conservation of energy, can be fruitfully deployed as a virtual sensor of removed heat load into a variety of residential and industrial applications.

17/01934 Molten corium–concrete interaction: investigation of convective heat transfer in a pool with gas sparging

Bottin, M. *et al. Annals of Nuclear Energy*, 2016, 93, 35–42.

During a severe accident in a pressurized water reactor, corium may fall in the reactor pit and interact with concrete. The CLARA facility, financed by EDF, IRSN, GDF-Suez and CEA, has been designed to understand the heat transfer phenomena involved in the molten concrete–corium interaction (MCCI). The facility is composed of a pool of simulant liquids, percolated by air and internally heated by direct electrical current. It is in contact with several heat exchangers in order to maintain walls at a constant temperature and to measure local heat losses. The experiments performed aimed at studying the influence on heat transfer of liquid viscosity (varying from 1 to 10,000 mPa s by dissolution of hydroxyethyl cellulose in the water), air injection superficial velocities (ranging from 0 to 10 cm/s) on both horizontal and vertical walls, and pool length. After a literature review on the existing heat transfer experiments and correlations for two-phase (liquid–gas) flow, the CLARA experiments are described. Then, the results obtained are presented: influence of superficial gas velocity and liquid properties (especially viscosity) on heat transfer, evaluation of ratio between heat transfer on vertical and horizontal interface, influence of the pool dimensions. Finally, the analysis and interpretation of CLARA experiments are given: comparison to the literature data, development of correlations concerning the heat transfer along the vertical and horizontal plate, comparison to results obtained with real materials. The results show that the presence of bubbles enhances heat exchange while an increasing viscosity lowers the heat transfer. The MCCI isotropic trends are different from those observed with prototypical materials suggesting that phenomena occurring at the corium–concrete interface are more complex than the ones present in CLARA experiments.

17/01935 Multiscale modelling for the thermal creep analysis of PCM concrete

Mohaine, S. *et al. Energy and Buildings*, 2016, 131, 99–112.

The requested thermal efficiency for new buildings leads to use new materials. In recent years, many researchers have conducted studies on the phase change materials (PCM) concrete composite. Fire safety in buildings has become an important requirement and building materials should have good fire behaviour in order to be used in certain applications. However, there are not many studies on the fire behaviour of PCM concrete. Therefore, the main goal of this study is to develop a numerical multiscale approach to simulate the thermo-mechanical behaviour at high temperatures of concrete containing microencapsulated PCM. An investigation was also conducted on the effect of the thermo-mechanical properties of shell materials used to encapsulate the PCM. PCM have been taken into account explicitly in modelling by considering their size distribution in a representative elementary volume. The effective thermo-mechanical parameters of the cement paste and the concrete have been calculated by a numerical homogenization method. Coupled thermal and mechanical loads have then been applied to the concrete with 10% and 15% of PCM at high temperatures. The use of melamine formaldehyde, with a Young's modulus of 4.5 GPa, and a particular curve of thermal expansion coefficient instead of polymethyl methacrylate as shell material, showed a better thermo-mechanical behaviour at high temperatures. The thermal deformation and the damage of the resultant PCM concrete were found to be acceptable for building use.

17/01936 Nanoadditives induced enhancement of the thermal properties of paraffin-based nanocomposites for thermal energy storage

Owolabi, A. L. *et al. Solar Energy*, 2016, 135, 644–653.

Nanocomposites of a paraffin wax base containing various concentrations (0.5, 1.0, and 1.5 wt%) of the aluminium, copper, zinc and iron nanoadditives were investigated experimentally and theoretically. The experimental results revealed that an increased weight percent of the additives, within the investigated range, enhanced the thermal properties for TES application. Adding 1.5 wt% of Cu and Zn nanoparticles enhanced the thermal conductivity of the nanocomposite by 20.6% and 61.5%, respectively. The thermal diffusivity was observed to increase proportionally as the thermal conductivity increases, whereas the specific heat decreases. The experimental results were compared with existing models, and they disagreed with the prediction results of the thermal conductivity values for all of the models in the literature. The Maxwell and Hamilton-Crosser models predicted the closest values to the experimental results; however, they underpredicted the thermal conductivity of the nanocomposite, whereas the values from the other models significantly overpredicted the thermal conductivity values. The collector efficiency performance was enhanced by 15.5% when integrated with PCM-TES. A further enhancement was reported when the collector system was integrated with nanocomposite-TES. The enhanced PCM nanocomposites exhibited improved thermal energy storage capability, mainly in solar/TES integrated applications.

17/01937 Natural circulation heat transfer model development over vertical tube bundle in the condensate heat exchanger

Chung, Y. J. *et al. Annals of Nuclear Energy*, 2016, 94, 759–766.

A 330 MWt integral type nuclear power plant, SMART, was developed for electricity generation and seawater desalination. Advanced design concepts were adopted such as an integral arrangement of the major components, and a passive residual heat removal system (PRHRS) to enhance the safety capability. The TASS/SMR code was developed using various thermal-hydraulic models reflecting the design features of SMART, such as the condensate heat exchanger in the passive residual heat removal system. The development and validation of the condensate heat exchanger model were performed using POSTECH and IIT heat transfer test results. The TASS/SMR code predicted well or slightly under-predicted the heat transfer coefficient at the condensate heat exchanger shell side compared with the experimental data. The heat transfer correlation considering the tube bundle effect improved the prediction of the heat transfer for a vertical tube bundle geometry.

17/01938 Natural convection effects in the heat transfer from a buried pipeline

di Schio, E. R. *et al. Applied Thermal Engineering*, 2016, 102, 227–233.

This study investigates the effect of the buoyancy on the heat transfer from a buried pipeline. The soil surrounding the pipe is modelled as a porous medium saturated by water, and the Darcy's law is assumed. Reference is made to a time-varying temperature distribution on the soil surface, and uniform and constant temperature on the pipe wall. The steady state regime is investigated as particular case. The heat power per unit length is evaluated for different values assumed by the Darcy–Rayleigh number, thus revealing that, for high values of *Ra*, the natural convection effects are non-trivial. A comparison with the case of pure conduction is made for the limiting case of a vanishing value of *Ra*, revealing an excellent agreement.

17/01939 $NiCoO_2$ flowers grown on the aligned-flakes coated Ni foam for application in hybrid energy storage

Xu, X. *et al. Journal of Power Sources*, 2016, 329, 238–246.

Many $NiCoO_2$ flowers with an average diameter of about 4 μm were grown on the $NiCoO_2$ flakes coated Ni foam (denoted as $NiCoO_2$/Ni foam) through a simple hydrothermal method and confirmed by scanning and transmission electron microscopies, X-ray diffraction and X-ray photoelectron spectrum measurements. The $NiCoO_2$/Ni foam with high specific area and porosity was directly used as the working electrode without any binders. The measured specific capacitance of $NiCoO_2$ grown on Ni foam is 756 F/g at 0.75 A/g using a three-electrode setup in 1 M KOH. Considering the high capacity of $NiCoO_2$ and the good stability of rGO, the $NiCoO_2$/Ni foam//rGO hybrid super-capacitor combining $NiCoO_2$/Ni foam and rGO shows very good properties, such as high specific capacitance (82 F/g at 2 A/g based on the total mass of active materials), high energy density (25.7 Wh/kg at 1500 W/kg based on the total mass of active materials), good stability (about 90% capacitance retention after 2000-cycle at 100 mV/s), and low charge ion transfer resistance.

17/01940 Normalized charging exergy performance of stratified sensible thermal stores

Njoku, H. O. *et al. Solar Energy*, 2016, 136, 487–498.

This paper presents the performance assessment of stratified sensible thermal energy stores (SSTES) on the basis of the normalized exergy efficiency, $\bar{\eta}_x$. Assessments based on $\bar{\eta}_x$ provide comparisons with performances of both the perfectly stratified and the fully mixed stores, which offer the best and worst performances, respectively. This is in contrast with energy and exergy efficiencies, which compare SSTES with only the perfectly stratified store. A dimensionless unsteady axi-symmetric model of vertical cylindrical SSTES was implemented using a finite volume numerical scheme. The effect of some significant parameters on SSTES performance were considered by performing computations for aspect ratios (AR) between 1 and 4, Peclet number (Pe_D) varying from 5×10^3 to 100×10^3, Richardson number (Ri) varying from 10 to 10^4, and overall heat loss coefficients (U) varying from 0 to 100 $W m^{-2} K^{-1}$. $\bar{\eta}$ increases with Pe_D, Ri and AR, with the most significant increases occurring at low values of these parameters, and appreciable increases are no longer obtained beyond $Pe_D \approx 30 \times 10^3$, $Ri \approx 10^3$ and AR ≈ 3. $\bar{\eta}_x$ also falls monotonically as the U values increase.

17/01941 Numerical optimization and experimental testing of a new low pressure heat exchanger (LoPHEx) for passive ventilation of buildings

Simonetti, M. *et al. Applied Thermal Engineering*, 2016, 103, 720–729.

Reducing primary energy consumption is an essential issue for the sector of building construction. This paper refers to building ventilation systems and focuses on low pressure flat plate heat exchangers, designed for low pressure drops and low air velocity, minimizing the electrical consumption of fans. The device is conceived for working within passive ventilation systems, as a ventilation heat recovery stage during winter and sensible heat dissipation during summer. Computational fluid dynamics simulations are used for testing and optimizing some flow-mixing device (or turbulators) inside the heat exchanger, in order to minimize the need for fans, still assuring an acceptable efficiency. Experimental testing of the prototype is in good agreements with numerical simulations.

17/01942 Numerical study of pressure drop and heat transfer from circular and cam-shaped tube bank in cross-flow of nanofluid

Lavasani, A. M. and Bayat, H. *Energy Conversion and Management*, 2016, 129, 319–328.

Flow and heat transfer of a nanofluid inside circular and cam-shaped tube bank is studied numerically. Reynolds number for cam-shaped tube bank is defined based on equivalent diameter of circular tube and varies in range of $100 \leq Re_D \leq 400$. The nanofluid is made by adding Al_2O_3 nanoparticles to a volume fraction of 1–7% to pure water. Experiment shows that using the nanofluid results in a higher heat transfer rate for both the circular tube bank and the cam-shaped tube bank. Also, a staggered arrangement has a higher heat transfer for both the circular and cam-shaped tube banks. The pressure drop from the cam-shaped tube bank is substantially lower than the circular tube bank for the whole range of Reynolds numbers and volume fractions.

17/01943 Optimal design of ionic liquids for thermal energy storage

Mehrkesh, A. and Karunanithi, A. T. *Computers & Chemical Engineering*, 2016, 93, 402–412.

Ionic liquids (ILs) are an emerging group of chemicals which, with their tunable physicochemical properties, exhibit promise for use as novel materials in many applications. Thermal (e.g. solar) energy storage is one such area where they show potential to be thermally stable at high temperatures and store high amount of heat energy. A large number of ILs, through the combination of different cations and anions, can be potentially synthetized thereby presenting a good platform for design. However, since it is not possible to study this large number of compounds experimentally it is necessary to use computational methods to evaluate them. Here the authors present a computer-aided framework to design task-specific ILs, using structure-property models and optimization methods. Thermal energy storage density (capacity) was used as a measure of the ability of an IL to store thermal (solar) energy. An hydroxyl functionalized imidazolium-based IL, $[3\text{-hydroxy-imidazolium}]^+[BF4]^-$, was found to be the optimal candidate with highest thermal energy storage capacity along with appropriate melting point and decomposition temperature.

17/01944 Performance improvement of a falling-film-type heat exchanger by insertion of shafts with screw blade in a heat exchanger tube

Shiraiwa, H. and Kita, Y. *Applied Thermal Engineering*, 2016, 102, 55–62.

Highly efficient heat exchange is expected for the falling-film-type heat exchanger handled in this study by utilizing a falling liquid film, etc. The heat medium is flowed inside the heat exchanger tube. In contrast, the falling film is flowed outside the heat exchanger tube, thereby exchanging heat. In the previous study, considering the basic heat transfer characteristic of the falling-film-type heat exchanger, the design equation was developed in the limited extent. In this study, focusing on the flow condition in a heat exchanger tube of the falling-film-type heat exchanger, various shafts with screw blade were inserted in a single heat exchanger tube and it was evaluated how the pitch and height of screw and the flow rate of cooling water would give an effect on the heat exchange performance. Additionally, the heat transfer coefficient and the overall heat transfer coefficient of the falling-film-type heat exchanger were logically calculated, and then a theoretical value and an experimental value were compared and evaluated. As a result, it was clarified that the heat exchange performance of the falling-film-type heat exchanger was improved by inserting the shaft with screw blade, and theoretical and experimental values were roughly matched.

17/01945 Performance of two mixed refrigerant processes providing refrigeration at 70 K

Narayanan, V. and Venkatarathnam, G. *Cryogenics*, 2016, 78, 66–73.

Mixed refrigerant process refrigerators are ideal for use in superconducting transformers, fault current limiters, etc. placed in a liquid nitrogen bath. Traditional mixed refrigerant processes used above 70 K cannot be used in these applications. The performance of two mixed refrigerant processes suitable for the above applications has been studied, the results of which are presented in this paper.

17/01946 Polymeric foams for cryogenic temperature application: temperature range for non-recovery and brittle-fracture of microstructure

Park, S.-B. *et al. Composite Structures*, 2016, 136, 258–269.

In the present study, low-temperature material characteristics of polyurethane foam, glass fibre-reinforced polyurethane foam, and polyisocyanurate foam were investigated. These foams are key candidate materials for use in membrane-type liquefied natural gas (LNG) insulation systems. LNG insulation systems should be able to withstand severe environmental conditions, such as fluid-induced impact loading under cryogenic temperatures. For the robust design of insulation system, both failure characteristics and deformation recovery capacity of the materials must be evaluated. Therefore, the failure characteristics and the deformation recovery ratio of the foams were investigated at various temperatures and strain rate levels. The present study revealed that the fracture behaviour and the recovery ratio were significantly affected by decreases in temperature. As a newly obtained insight, it has been found that the recovery ratio for all tested materials significantly decreased at −163 °C. This finding is the opposite of the behaviour that typically occurs at low temperatures. In particular, polyurethane foam specimen after experiment at the temperature of −163 °C was easily broken into pieces even under the application of small loads. In addition, it has been revealed that polyisocyanurate foam showed superior mechanical characteristics at cryogenic temperatures owing to the ring structure of isocyanurate.

17/01947 Preparation and thermal properties of n-octadecane/stearic acid eutectic mixtures with hexagonal boron nitride as phase change materials for thermal energy storage

Su, D. *et al. Energy and Buildings*, 2016, 131, 35–41.

This work focuses on preparing *n*-octadecane (ODE) and stearic acid (SA) eutectics which contain hexagonal boron nitride (HBN) to improve thermal conductivity of the composites. In the composites, the SA–ODE eutectic mixtures acted as phase change materials (PCMs) for thermal energy storage, the HBN was introduced to enhance the thermal conductivity. Analysis methods such as Fourier transformation infrared spectroscopy, X-ray diffraction and scanning electronic microscopy were used to test the chemical bonding, crystalloid phase and morphology of the eutectic mixture/hexagonal boron nitride composites. The thermal properties, thermal stability and thermal conductivity were measured by differential scanning calorimetry, thermogravimetric analysis and thermal conductivity, respectively. It was shown that there was no chemical reaction between the SA–ODE eutectic and HBN, and the composite PCMs (CPCMs) had good thermal stability. The thermal conductivities of the melted/solidified CPCMs increased because of adding HBN, whereas their latent heat of fusion slightly decreased. The SA–ODE eutectic with 10 wt% HBN was chosen as satisfactory CPCM. It melted at 27.89 °C with the latent heat of 207.6 kJ/kg and solidified at 26.53 °C with the latent heat of 202.05 kJ/kg. It is envisioned that the prepared SA–ODE/HBN composites have application prospect as PCMs in thermal energy storage.

17/01948 Quantifying the operational flexibility of building energy systems with thermal energy storages

Stinner, S. *et al. Applied Energy*, 2016, 181, 140–154.

The increasing share of fluctuating renewable energy generation in the energy system increases the need for flexibility options. Building energy systems (BES) with their corresponding thermal energy storages (TES) can be one option for supplying flexibility. To use this option efficiently, a framework to quantify the flexibility of the BES is necessary. It is found that the flexibility of a BES can hardly be described with one single flexibility indicator. Therefore, this paper develops a method to analyse the flexibility of BES in terms of time, power and energy. Different influencing factors are considered, like the heat generator and the thermal storage size. Additionally, the option to aggregate the different flexibility measures on a city district level is addressed. This is necessary as single buildings have a minor impact on higher level energy systems. Finally, a comparison to other flexibility options like battery storage is discussed.

17/01949 Radiation heat transfer in high porosity open-cell metal foams for cryogenic applications

Dixit, T. and Ghosh, I. *Applied Thermal Engineering*, 2016, 102, 942–951.

Radiation heat transfer in high porosity open-cell metal foams subjected to cryogenic temperatures has been studied. This study helps designing metal-foam-based devices exposed to radiation of deep space at extremely low temperature. Aluminium and copper foam samples with more than 90% and 95% void volume respectively and pore size in the range of 10–30 PPI have been studied. Suspending the foam samples freely inside a vacuum chamber (at 10^{-6} mbar) and maintaining the chamber wall at liquid nitrogen temperature, the cool down time–temperature profiles has been recorded for nearly 5.5 h, wherein different foams reach temperatures in the range of 119–128 K. Simultaneously, theoretical model based on lumped-capacity analysis has been developed to simulate the transient behaviour of foam samples. Simple cubic structure foam model has been used to estimate the view factor. The experimental outcome could be predicted by the theoretical model with reasonable accuracy. Additionally, cool-down history of an aluminium foam sample has been compared to a solid body of same weight so as to appreciate their radiative potential at low temperatures.

17/01950 Sequential synthesis of heat integrated water networks: a new approach and its application to small and medium sized examples

Jagannath, A. and Almansoori, A. *Computers & Chemical Engineering*, 2016, 90, 44–61.

This paper presents a new step-wise sequential solution strategy for the synthesis of heat integrated water networks (HIWNs) comprising of two mathematical models. The first model minimizes water and energy costs. The optimal freshwater and water flow rates within the HIWN are determined from this model. Using these optimal flow rates, different configurations of HIWN are evaluated for the purpose of heat integration. The second model is the stage-wise heat exchanger network which is solved for each of the evaluated network configuration in a sequential manner. Using this proposed strategy, a set of locally optimal HIWNs are produced and the best one is chosen based on the minimum total annual cost. The proposed sequential strategy is applied to small- and medium-sized examples in the literature. The results show that the proposed new sequential solution strategy can be successfully applied to small and medium sized HIWN problems.

17/01951 Temperature determination of tilted electronic assemblies equipped with basic and wire-bonded QFN16 and 32 devices subjected to free convection

Baïri, A. *Applied Thermal Engineering*, 2016, 102, 565–569.

The correlations proposed in this work allow the calculation of the average temperature on different areas of electronic assemblies containing basic QFN16 and QFN32 packages and their wire-bonded versions named QFN16b and QFN32b, respectively. The study is based on correlations proposed in recent works allowing calculation of the average natural convective heat transfer coefficient according to the power generated by the package and the tilt angle of the printed circuit board (PCB) on which they are welded. The considered generated power is within the range 0.1–1 W for the QFN16 and 16b models. For the QFN32 and QFN32b, the correlations are extended to lower power ranging from 0 (off) to 0.1 W. These power ranges are associated to an inclination angle of the PCB varying between 0° and 90° (horizontal and vertical positions respectively) corresponding to the operative conditions of these devices increasingly used in electronics. Temperature determination of every part of these assemblies through the proposed correlations easy to use, helps improving their thermal design and reliability.

17/01952 Thermal conductivity of a new carbon nanotube analog: the diamond nanothread

Zhan, H. *et al. Carbon*, 2016, 98, 232–237.

Based on the non-equilibrium molecular dynamics simulations, the authors have studied the thermal conductivities of a novel ultra-thin one-dimensional carbon nanomaterial – diamond nanothread (DNT). Unlike single-wall carbon nanotube (CNT), the existence of the Stone-Wales (SW) transformations in DNT endows it with richer thermal transport characteristics. There is a transition from wave-dominated to particle-dominated transport region, which depends on the length of poly-benzene rings. However, independent of the transport region, strong length dependence in thermal conductivity is observed in DNTs with different lengths of poly-benzene ring. The distinctive SW characteristic in DNT provides more to tune the thermal conductivity not found in the homogeneous structure of CNT. Therefore, DNT is an ideal platform to investigate various thermal transport mechanisms at the nanoscale. Its high tunability raises the potential to design DNTs for different applications, such as thermal connection and temperature management.

17/01953 Thermal properties improvement of lithium nitrate/graphite composite phase change materials

Lachheb, M. *et al. Applied Thermal Engineering*, 2016, 102, 922–931.

This paper addresses the development and the thermal investigation of new composite materials with improved thermo-physical properties destined for solar thermal energy storage at high temperature. The thermo-physical properties of composites are characterized by using several techniques based on the temperature measurement and the obtained results are compared to the theoretical values calculated by different analytical models. The results of these experiments revealed a clear improvement in the different thermal properties when integrating graphite particles in the composite. In the other hand, a good agreement between experimental and theoretical values was obtained.

17/01954 Thermochemical heat storage materials – performance of mixed salt hydrates

Rammelberg, H. U. *et al. Solar Energy*, 2016, 136, 571–589.

Thermochemical heat storage is highly promising, in particularly with a view to long-term heat storage. For the implementation of heat storage in households, thermochemical reactions in the low temperature range below 120 °C are important. Especially salt hydrates such as $MgCl_2$, $CaCl_2$ or $MgSO_4$ were tested with micro gravimetric methods for their suitability. However, the cycle stability of consecutive charging (dehydration) and discharging (hydration) reactions of these materials was low and could be improved only by control of the water uptake (i.e. discharging time) to prevent overhydration. In contrast, mixtures of these salt hydrates showed significant improvements in cycle stability, mass and enthalpy balances. The experiments also showed that the cycleability of all investigated materials increased if hydration and dehydration reactions were performed under constant vapour pressure of 21 mbar. Contrary to other materials, the mixture of $CaCl_2$ and $MgCl_2$ showed good cycleability under all tested conditions. In addition, the mixture showed superior kinetic properties. Additionally, there is evidence of tachyhydrite ($CaMg_2Cl_6 \cdot 12H_2O$) formation during cycling of the mixture by the use of X-ray diffraction after the thermal analysis. Further investigations will be performed to identify further synergies, ideal mixing ratios and formed phases.

17/01955 Two-phase optimizing approach to design assessments of long distance heat transportation for CHP systems

Hirsch, P. *et al. Applied Energy*, 2016, 182, 164–176.

Cogeneration or combined heat and power (CHP) for power plants is a method of putting to use waste heat which would be otherwise released to the environment. This allows the increase in thermodynamic efficiency of the plant and can be a source of environmental friendly heat for district heating (DH). In this paper, CHP for nuclear power plants (NPP) is analysed with the focus on heat transportation. A method for effectivity and feasibility evaluation of the long distance, high power heat transportation systems (HTS) between the NPP and the DH network is proposed. As a part of the method the multi-criteria decision-making problem, having the structure of the mathematical programming problem, for optimized selection of design and operating parameters of the HTS is formulated. The constraints for this problem include a static model of HTS, that allows considerations of system lifetime, time variability and spatial topology. Thereby variation of annual heat demand within the DH area, variability of ground temperature, insulation and pipe aging and/or terrain elevation profile can be taken into account in the decision-making process. The HTS construction costs, pumping power, and heat losses are considered as objective functions. In general, the analysed optimization problem is multi-criteria, hybrid and non-linear. The two-phase optimization based on optimization-simulation framework is proposed to solve the decision-making problem. The solver introduces a number of assumptions concerning the optimization process. Methods for problem decomposition, scalarization and relaxation are proposed and optimization procedures for the decomposed problem are discussed. The methodology is tested on a sample case study of the NPP planned to be built in northern Poland. The sensitivity analysis of the problem is also provided.

17/01956 Visualization of the solid–liquid equilibria for non-flammable mixed refrigerants

Lee, C. *et al. Cryogenics*, 2016, 75, 26–34.

Non-flammable mixed refrigerant (NF-MR) Joule–Thomson (J–T) refrigerators have desirable characteristics and wide cooling temperature range compared to those of pure J–T refrigerators. However, the operating challenge due to freezing is a critical issue to realize this type of refrigerator. In this paper, the solid–liquid phase equilibria (i.e. freezing point) of the NF-MR which is composed of argon (Ar), R14 (CF_4), and R218 (C_3F_8), has been experimentally investigated by a visualized apparatus. The accuracy of the apparatus is experimentally verified with pure refrigerants and selected binary mixed refrigerants. Freezing points of the ternary NF-MRs have been measured with the molar compositions from 0.1 to 0.8 for each component. Each test result is simultaneously acquired by a camcorder for visual inspection and temperature measurement during a warming process. Experimental results reveal that the specific MR, with R14 molar composition

higher than 0.4, can achieve remarkably low freezing temperature even below 77 K. These unusual freezing point depression characteristics of the MR can be a useful information for designing a cryogenic MR J–T refrigerator to reach temperatures less than 77 K.

11 ENGINES

Power generation and propulsion, electrical vehicles

17/01957 A comparative study on influence of fuel additives with edible and non-edible vegetable oil based on fuel characterization and engine characteristics of diesel engine

Shah, P. R. and Ganesh, A. *Applied Thermal Engineering*, 2016, 102, 800–812.

Use of vegetable oil as compression ignition engine fuel has been investigated by many researchers during last decade either by direct blending with diesel or converting it into bio-diesel but very few publications available regarding its direct use in engine. The direct use of straight vegetable oil leading to formation of injector deposits which in turn produces higher exhaust emissions. Fuel improvement through additive is an attractive option in existing diesel engine without any modification to meet worldwide legislative efforts to lower airborne pollution. Hence, use of locally available vegetable oil with addition of fuel additive in existing diesel engine becomes an indispensable tool in global trade to meet ever-tightening pollutant emissions regulations for heavy-duty diesel engine. This paper intends to compare the behaviour of edible and non-edible crude vegetable oil on engine characteristics of existing diesel engine under similar operating condition with cognitive elaboration. The main purpose of the present work was to investigate how commercially available fuel additives for diesel fuel, influence the edible and non-edible vegetable oil, by comparing the combustion, emission and performance characteristics under similar operating condition. A comparative study was carried out on Cummins two cylinder DI diesel engine at constant speed by varying brake load. The Sunflower oil (SF) was selected as edible oil and Karanj oil (KO) as non-edible oil whereas two commercially available fuel additives for diesel referred as 'A1' and 'A2' respectively in this study were procured for test trial. The experimentally obtained results revealed that both edible oil (SF) and non-edible oil (KO) showed longer ignition delay which in turn leading to higher cylinder pressure, HRR, higher NO_x and CO emissions whereas showed lower BSEC and smoke opacity as compared to diesel fuel. However, the KO oil exhibited lower NO_x and CO emissions when compared to SF while maintaining marginal difference in thermal efficiency. The test results showed that both additives were found effective in reduction of ignition delay, HRR and NO_x formation with KO whereas increased NO_x and CO emissions with SF. The additive A1 significantly reduced CO and smoke emissions with KO while the opposite trend was observed when additive A2 was used.

17/01958 A predictive power management controller for service vehicle anti-idling systems without a priori information

Huang, Y. *et al. Applied Energy*, 2016, 182, 548–557.

This paper presents a model predictive power management strategy for a novel anti-idling system, regenerative auxiliary power system (RAPS), designed for service vehicles. RAPS is able to utilize recovered braking energy for electrified auxiliary systems; this feature distinguishes it from its counterparts – auxiliary power unit (APU) and auxiliary battery powered unit (ABP). To efficiently operate the RAPS, a power management strategy is required to coordinate power flow between different energy sources. Thus, a model predictive controller (MPC) is developed to improve the overall efficiency of the RAPS. As an optimization-based approach, the MPC-based power management strategy usually requires the drive cycle or the drivers' command to be known *a priori*. However, in this study, an average concept based MPC is developed without such knowledge. MPC parameters are tuned over an urban drive cycle; whereas, the robustness of this MPC is tested under different drive cycles (e.g. highway and combined). Analysis shows that, the presented MPC has a comparable performance as the prescient MPC regarding fuel consumption, which assumes knows the drive cycle beforehand. Meanwhile, with the help of the proposed MPC and RAPS, the service vehicle saves up to 9% of the total fuel consumption. The proposed MPC is independent of powertrain topology such that it can be directly extended to other types of hybrid electric vehicles, and it provides a way to apply the MPC even though future driving information is unavailable.

17/01959 A theoretical investigation of the effects of the low-temperature reforming products on the combustion of *n*-heptane in an HCCI engine and a constant volume vessel

Wang, Y. *et al. Applied Energy*, 2016, 181, 132–139.

A new concept of the flexible cylinder engine for the combustion in the engine cylinders is developed to optimize the combustion process, according to the practical working conditions. By the new concept, the fuel is reformed in the flexible cylinder, mixed with the same fresh fuel, and then introduced into the normal cylinders to finish the normal combustion process. The reformed fuel may alter the combustion reaction pathways of the fresh fuel and hence may improve the combustion in the engine cylinders potentially. In this work, the effects of the reformed fuel on the combustion of the fresh fuel were investigated by using *n*-heptane as the model fuel to demonstrate this new concept theoretically. It was found that the reformed fuel may decrease the ignition delay time of the fresh fuel by about 6° top dead crank angle at a typical engine condition. Among the reformed species, ketohydroperoxides and hydrogen peroxide are the key species to decrease the ignition delay time besides the radicals. The reformed fuel may increase the laminar flame speed of the fresh fuel, with H_2 and CO being the key species. Finally, the reformed fuel may also decrease the harmful emissions, such as the unburned hydrocarbons, including acetylene, ethylene, propyne, propylene, 1,3-butadiene and the partially oxidized species, including formaldehyde, ketone, acetaldehyde, etc. These simulation results indicate that the new concept of the flexible cylinder engine is a potential clean combustion strategy for the engines.

17/01960 Comparison of different gas turbine cycles and advanced exergy analysis of the most effective

Fallah, M. *et al. Energy*, 2016, 116, 701–715.

Four gas turbine systems are compared: simple gas turbine (SGT), gas turbine with evaporative inlet air cooler (EVGT), steam injection gas turbine (STIG) and steam injection gas turbine with evaporative inlet air cooler (ESTIG). These comparisons are done on the basis of conventional exergy analysis and the results show that the ESTIG cycle is the most advantageous for the designer. After determining the ESTIG optimum conditions from maximum net work and maximum second-law efficiency perspectives using conventional exergy analysis, advanced exergy analysis is performed for this system at its optimum conditions to provide detailed information about the improvement potential of the system components. The analysis is carried out on the basis of the engineering method and the thermodynamic cycle method is used to validate the endogenous exergy destruction rates of the system components. The results show that the optimization priority order for the system components is different when determined with advanced exergy analysis compared to conventional exergy analysis.

17/01961 Effect of split injections coupled with swirl on combustion performance in DI diesel engines

Li, X. R. *et al. Energy Conversion and Management*, 2016, 129, 180–188.

Engine-out emissions (NO_x and soot) have led to serious air pollution problems, and consequently, increasingly stringent emission norms. In order to decrease the emissions and improve the combustion performance of diesel engines, the effect of split injections with swirl (swirl rate of 0 and 1) was experimentally researched, and the mechanism of the fuel/air mixture of split injections with swirl (swirl rate of 0.5–2.5) was numerically researched in this study. The experimental research was carried out on a modified 1132Z single-cylinder diesel engine, equipped with an endoscope system. A two-colour method was applied to record flame temperature distribution and KL factor. The experimental results indicate that the flame observed using split injections with swirl rotated obviously. Split injections with swirl had a positive influence on improving the fuel/air mixture, accelerating combustion progress and shortening combustion duration. The combustion duration decreased at swirl rate of 1, with a reduction in the range of 19.5–25.7% at various pilot quantities. In addition, brake-specific fuel consumption (BSFC) and soot emission were reduced. BSFC was lower at swirl rate of 1 than that at swirl rate of 0, with a reduction in the range of 1.1–2.01 $g/(kW\,h)^{-1}$. For KL factor at 12° CA ATDC, it was also observed that at 12° CA ATDC, the KL factor was lower at swirl rate of 1 than that at swirl rate of 0, with a reduction of 34.9%. Related numerical research on split injections with swirl was performed, and the results show that at a specific swirl, the main injection deviated from the pilot injection and entered the area between two sprays, enhancing the utilization of air in the chamber. In addition, the main combustion process accelerated due to the better thermal-atmosphere provided by the pilot injection, so that a better engine performance and lower soot concentration was achieved.

17/01962 Energy distributions in a diesel engine using low heat rejection (LHR) concepts

Li, T. *et al. Energy Conversion and Management*, 2016, 130, 14–24.

The energy balance analysis is recognized as a useful method for aiding the characterization of the performance and efficiency of internal combustion (IC) engines. Approximately one-third of the total fuel energy is converted to useful work in a conventional IC engine, whereas the major part of the energy input is rejected to the exhaust gas and the cooling system. The idea of a low heat rejection (LHR) engine (also called the 'adiabatic engine') was extensively developed in the 1980s due to its potential in improving engine thermal efficiency via reducing the heat losses. In this study, the LHR operating condition is implemented by increasing the engine coolant temperature (ECT). Experimentally, the engine is overcooled to low ECTs and then increased to 100 °C in an effort to get trend-wise behaviour without exceeding safe ECTs. The study then uses an engine simulation of the conventional multi-cylinder, four-stroke, 1.9 L diesel engine operating at 1500 rpm to examine the five cases having different ECTs. A comparison between experimental and simulation results show the effects of ECT on fuel conversion efficiency. The results demonstrate that increasing ECT yields slight improvements in net indicated fuel conversion efficiency, with larger improvements observed in brake fuel conversion efficiency.

17/01963 Experimental investigation of a diesel engine power, torque and noise emission using water–diesel emulsions

Seifi, M. R. *et al. Fuel*, 2016, 166, 392–399.

This study reports the results of an investigation on a Perkins A63544 direct injection diesel engine using water–diesel emulsions (2%, 5%, 8% and 10% water by volume). The engine was run at different engine speeds ranging from 1400 to 1900 rpm, with steps of 100 rpm, for power and torque analysis. In order to evaluate noise emissions, four engine speeds (1600–1900 rpm with steps of 100 rpm) and four engine load conditions (25%, 50%, 75% and 100%) were selected. No change in engine components and fuel injection systems was made. The statistical analysis results showed that the engine speed and fuel type parameters had significant effects at 1% probability level ($P < 0.01$) on the average values of the engine power and torque. The engine noise emission was affected significantly ($P < 0.01$) by the engine speed, fuel type and engine load parameters. The results showed that adding small amounts of water, 2%, to neat diesel fuel produced a significant increase in the engine power. Furthermore, its engine torque and noise emission were comparable with those of neat diesel fuel. The higher water addition to diesel decreased the engine power and torque, however no such change was found for the engine noise emission. The significant increase in the engine power and comparable engine torque and noise emission for 2% water content showed a good potential for this emulsion to be considered as an appropriate alternative to neat diesel fuel.

17/01964 Experimental investigations of effects of EGR on performance and emissions characteristics of CNG fueled reactivity controlled compression ignition (RCCI) engine

Singh Kalsi, S. and Subramanian, K. A. *Energy Conversion and Management*, 2016, 130, 91–105.

Experimental tests were carried out on a single-cylinder diesel engine (7.4 kW rated power at 1500 rpm) under dual fuel mode [compressed natural gas (CNG)–diesel] with exhaust gas recirculation (EGR). Less reacting fuel (CNG) was injected inside the intake manifold using timed manifold gas injection system whereas high reactive diesel fuel was directly injected into the engine's cylinder for initiation of ignition. EGR at different percentages (8%, 15% and 30%) was inducted to the engine through intake manifold and tests were conducted at alternator power output of 2 and 5 kW. The engine can operate under dual fuel mode with maximum CNG energy share of 85% and 92% at 5 and 2 kW, respectively. The brake thermal efficiency of diesel engine improved marginally at 5 kW power output under conventional dual fuel mode with the CNG share up to 37% whereas the efficiency did not change with up to 15% EGR however it decreased beyond the EGR percentage. NO_x emission in diesel engine under conventional dual fuel mode decreased significantly and it further decreased drastically with EGR. The notable point emerged from this study is that CO and HC emissions, which are major problems at part load in reactivity controlled compression ignition engine (RCCI), decreased with 8% EGR along with further reduction of NO_x. However, smoke emission is marginally higher with EGR than without EGR but it is still less than conventional mode (diesel alone). The new concept emerged from this study is that CO and HC emissions of RCCI engine at part load can be reduced using EGR.

17/01965 Fuelling of spark ignition and homogenous charge compression ignition engines with low calorific value producer gas

Przybyla, G. *et al. Energy*, 2016, 116, 1464–1478.

The present paper summarizes results of experimental trails with the SI and HCCI engine fuelling with a producer gas substitute. Both engines are single cylinder units with similar displacement volume. In its original version, the HCCI engine used to be a three cylinder CI engine. Two of those cylinders were disabled when the engine was modified for the HCCI operation. The SI engine used in this was a component of commercially available generator. The engine original intake manifold and ignition system were rebuild for the purpose of this study. Engines were fuelled with the producer gas substitute that simulated real producer gas composition. The SI engine was charged with a stoichiometric air/fuel mixture, while the HCCI engine with a lean air/fuel mixture with equivalence ratio of 0.5. The main control variable in the SI engine operation was the spark timing. The initial air preheat temperature was the equivalent control variable in the HCCI engine trials. This paper reports on both engines indicated performance and combustion phasing parameters that were derived based on in-cylinder, cycle resolved pressure measurements.

17/01966 Heat transfer in premixed spark ignition engines part II: systematic analysis of the heat transfer phenomena

De Cuyper, T. *et al. Energy*, 2016, 116, 851–860.

The heat transfer is a keystone sub-model for engine simulation tools since it affects all targeting parameters (power output, efficiency and emissions. Part I of this work reported a thorough review of heat transfer measurements from literature. Using design of experiments, two measurement matrices were constructed, one for motored and one for fired operation. The present paper focuses on the measurements under fired operation and analyses the heat transfer phenomena in a systematic way. First, the effect of the dependent engine settings on the heat flux is analysed in a consistent way using analysis of variance. Second, it also discusses the influence of the gas properties on the heat flux, which has been overlooked by many authors. Third, the validity of the Reynolds analogy modelling approach is checked, and several improvements are proposed.

17/01967 Impulse control method for hydraulic propulsion system used in 3500 m work-class ROV

Huo, X. *et al. Applied Ocean Research*, 2016, 60, 75–83.

In terms of the non-linear characteristics of hydraulic propulsion system used in 3500 m rated work-class remotely operated underwater vehicle, the paper improved the responsiveness of the hydraulic propulsion system by adding an impulse signal to the input end of the system. Because the maximum static damping moment provided from water is much larger than the dynamic damping moment, it results in large dead zone of thrust during the start-up process of the hydraulic propulsion system. The dead zone of thrust caused by static damping moment can be effectively reduced by adding a specific impulse signal to the input end of the propulsion system. The results of numerical simulations and underwater experiments show that using this method, the non-linear characteristics of the hydraulic propulsion system have been significantly improved.

17/01968 Investigation of transient deterioration mechanism and improved method for turbocharged diesel engine

Han, Y. *et al. Energy*, 2016, 116, 250–264.

The object of this paper is to reveal the mechanism of combustion process and pollutant emission deterioration during transient operation and propose an improve method to reduce transient smoke opacity as much as possible while keep NO_x formation below steady state condition. The paper reveals the transient operation deterioration mechanism from the following three levels. First, the combustion parameters response level (also known as boundary condition response level). Second, combustion process level (chiefly refer to apparent heat release rate, in-cylinder pressure, combustion phasing and combustion duration, etc.). Third, in-cylinder micro-analysis level (chiefly refer to air–fuel mixing energy). The main contributor of performance deterioration is boundary conditions deviation which caused by inconsistent response delay due to turbocharger lag. The consequence of boundary condition deviation is air–fuel mixing energy reduction. The improved method is to increase air–fuel mixing energy to compensate the negative effect cause by turbocharged lag. This work increases mixing energy by means of advancing injection timing. The results indicates that: the BTE increases 2.2% and smoke decreases 12.1% as the injection timing advances 2° CA, compared with the level under original injection timing. Therefore increasing mixing energy can alleviate transient operation deterioration by improving the quality air–fuel mixture formation.

17/01969 Optimization of dual-loop exhaust gas recirculation splitting for a light-duty diesel engine with model-based control

Park, J. and Choi, J. *Applied Energy*, 2016, 181, 268–277.

The objective of this research was to develop dual-loop exhaust gas recirculation (EGR) split strategies. Model-based control was performed by coupling one-dimensional (1D) cycle simulation with control logic, and the EGR split index (ESI) was developed to investigate split effects on performance and emission. The key control logic concept was to compensate the low pressure EGR rate. Additionally, ESI, a newly developed index, is a non-dimensional factor expressing the high pressure and low pressure portions of the total EGR rate. Using the control model and ESI, the maximum EGR rates were determined under each operating condition, thereby maintaining lean burn combustion and minimizing NO_x emission. A multi-objective Pareto method was used with the model-based control to optimize the engine operating parameters and thereby minimize NO_x formation and fuel consumption. The control logic applied a step transient analysis based on the optimized parameters.

17/01970 Particulate emissions from hydrogen enriched compressed natural gas engine

Hora, T. S. *et al. Fuel*, 2016, 166, 574–580.

Compressed natural gas (CNG) and hydrogen enriched compressed natural gas (HCNG) have not been investigated extensively for particulate emissions, when they are used as fuel in the internal combustion (IC) engines. This study investigated the particulate emissions from spark ignition HCNG fuelled engine with varying fractions of hydrogen (0%, 10%, 20% and 30% v/v). Experiments were performed on a prototype single cylinder (1 L) port fuel injected HCNG engine at varying loads (BMEP), while maintaining identical fuel injection conditions, engine speed and ignition timing. At each operating point, exhaust samples were collected from the engine tail pipe and particle size-number distribution was determined using engine exhaust particle sizer (EEPS). Similar trend was observed for each HCNG composition. Results showed higher particulate numbers in nano-particle size range, but their corresponding mass contribution was rather small. On the other hand, accumulation and coarse mode particles were lower in particulate size-number distribution but they contributed dominatingly to the particulate size-mass distribution. Among the tested HCNG compositions, 30HCNG showed highest number of nano-particles emitted at each engine load amongst with corresponding higher contributions to size-mass and size-surface area distributions.

17/01971 Performance of a lab-scale tubular-type electrostatic precipitator using a diesel engine particle emission source

Crespo, B. *et al. Energy*, 2016, 116, 1444–1453.

Air pollution is a topic currently studied to address the well-known health problems that can arise from it. The use of an electrostatic precipitator (ESP) for treatment with submicron particles from sources such as small-scale combustion systems presents some advantages in comparison to other possible devices. In this study, a new ESP prototype geometry based on separating the discharge electrode support from the gas stream path was designed, constructed and tested. The gas stream from a small-size diesel internal combustion engine was used. Good ESP behaviour over moderate time periods was verified by achieving average collection efficiencies of $97 \pm 4\%$. Thermogravimetric and scanning electron microscopy with energy dispersive X-ray spectroscopy analyses were performed. The influence of the regulation power value and the discharge electrode effective length on the collection efficiency was evaluated. Higher removal efficiencies were linked to higher power values and higher discharge electrode effective lengths. A high impact of the operating time was observed. Different discharge electrode geometries were tested, indicating an increase in collection efficiency as the power increased for stainless steel electrodes and the opposite trend for M12 threaded rod electrodes.

17/01972 Performance, combustion timing and emissions from a light duty vehicle at different altitudes fueled with animal fat biodiesel, GTL and diesel fuels

Ramos, Á. *et al. Applied Energy*, 2016, 182, 507–517.

The altitude effect on performance, emissions and thermodynamic diagnosis under real world driving conditions has been evaluated using two alternative fuels and a diesel fuel. Three places, at different altitudes, were selected for the tests, from 0 to 2500 m above the sea level. Besides, two type of circuits (urban and extra-urban) have been selected in order to evaluate these two driving pattern conditions. A light duty diesel vehicle equipped with the same after-treatment system as Euro 5 engines was used as test vehicle. Thermodynamic diagnosis shows that, when the engine works with two pre-injection events (mainly at high altitude and without exhaust gas recirculation) the ignition delay agrees of the cetane number of fuels. At urban conditions, altitude increases the combustion duration of all fuels and particularly with paraffinic fuels. The effect of altitude on THC and CO emissions is not noticeable, but at high altitude, NO_x emissions during extra-urban tests were around three times higher than those from testing along the urban circuit. Besides, compared to circuits next to the sea level, these emissions at both circuits (urban and extra-urban) were around 10 times higher, respectively, than the limits established by the Euro standards. The effect of fuels on pollutant emissions was masked by the variability associated to real driving conditions.

17/01973 Robust sliding mode control of a mini unmanned underwater vehicle equipped with a new arrangement of water jet propulsions: simulation and experimental study

Zakeri, E. *et al. Applied Ocean Research*, 2016, 59, 521–542.

This paper presents dynamical modelling and robust control of a mini unmanned underwater vehicle (MUUV) equipped with a new arrangement of water jet propulsion. The water jet propulsion includes some advantages comparing with a propeller one, such as, reducing the number of required motors, desired number and arrangement of the propulsions, removing adverse torque and cavitation due to propeller rotation and etc. In order to model the proposed MUUV, the gray box method is used in such a way that the dynamical equation of motion is derived analytically by Euler–Lagrangian method, and then the hydrodynamic coefficients (such as added mass and drag coefficients) are derived by performing some tests in a computational fluid dynamic software. The dynamical model is used to simulate the MUUV system and also to design the proposed controllers, which are feedback linearization controller (FLC) and sliding mode controller (SMC). In order to investigate and compare the performance of the MUUV and the applied controllers, three types of tests including a desired signal tracking case and two desired path-tracking cases are designed. To do so, a method is presented to obtain the desired signals from a desired path under predetermined conditions. Then, an MUUV prototype is designed and constructed in order to investigate the performance of the proposed water jet propulsions and controllers for regulation and tracking desired signal purpose, experimentally. As it is expected, the simulation and experimental results show better performance of the SMC compared to FLC. Furthermore, the experimental results reveal that the water jet propulsion is implementable to practical prototypes and also can be produced in an industrial level.

17/01974 The spark spread and clean spark spread option based valuation of a power plant with multiple turbines

Elias, R. S. *et al. Energy Economics*, 2016, 59, 314–327.

This paper offers a novel study of two key factors that affect the valuation of a natural gas-fired power plant having multiple turbines: carbon allowance prices and the ability to switch among turbines. Amid stricter environmental rules on CO_2 emissions, a power plant operator needs to be able to judge how the purchase of carbon allowances affects the plant's expected value; and whether the plant's value rises from switching among turbines. This paper presents a model analysis of a spark spread and clean spark spread option-based valuation of a power plant with multiple gas turbines – using a bivariate and a trivariate lattice, respectively. Results demonstrate that the purchase of CO_2 allowances lowers the plant's expected value. Conversely, when operations of turbines are switched in response to price movements, the plant's value increases. This outcome has implications for plant management decisions: when to switch among turbines and how the purchase of CO_2 allowances affects the plant's value.

17/01975 Transient stress control of aeroengine disks based on active thermal management

Ding, S. *et al. Applied Thermal Engineering*, 2016, 103, 16–27.

The physical essence of cooling in the turbine system is a process of thermal management. In order to overcome the limits of passive thermal management based on thermal protection, the concept of active thermal management based on thermal load redistribution has been proposed. On this basis, this paper focuses on a near real aeroengine disk during a transient process and studies the stress control mechanism of active thermal management in transient conditions by a semi-analytical method. Active thermal management is conducted by imposing extra heating energy on the disk hub, which is represented by the coefficient of extra heat flow η. The results show that the transient stress level can be effectively controlled by actively adjusting the thermal load distribution. The decline ratio of the peak equivalent stress of the disk hub can be 9.0% for active thermal management load condition ($\eta = 0.2$) compared with passive condition ($\eta = 0$), even at a rotation speed of 10,000 r/min. The reason may be that the temperature distribution of the disk turns into an artificial *V*-shape because of the extra heating energy on the hub, and the resulting thermal stresses induced by the negative temperature gradients counteract parts of the stress from rotating.

Hybrid engine systems

17/01976 A demand-side approach to the optimal deployment of electric vehicle charging stations in metropolitan areas

Andrenacci, N. *et al. Applied Energy*, 2016, 182, 39–46.

Despite all the acknowledged advantages in terms of environmental impact reduction, energy efficiency and noise reduction, the electric mobility market is below expectations. In fact, electric vehicles have limitations that pose several important challenges for achieving a sustainable mobility system: among them, the availability of an adequate charging infrastructure is recognized as a fundamental requirement and appropriate approaches to optimize public and private investments in this field are to be delineated. This paper considers actual data on conventional private vehicle usage in the urban area of Rome to carry out a strategy for the optimal allocation of charging infrastructures into portions (subareas) of the urban area, based on an analysis of a driver sample under the assumption of a complete switch to an equivalent fleet of electric vehicles. Moreover, the energy requirement for each one of the subareas is estimated in terms of the electric energy used by the equivalent fleet of electric vehicles to reach their destination. The model can be easily generalized to other problems regarding facility allocation based on user demand.

17/01977 A numerical investigation on combustion and emission characteristics of a dual fuel engine at part load condition

Mousavi, S. M. *et al. Fuel*, 2016, 166, 309–319.

Dual fuel engines are more attractive due to lower emission levels in comparison with conventional diesel engines particularly at full loads. But it is required to study dual fuel combustion process with more details at part loads due to the poor performance and high CO and UHC emissions at these conditions. In the present study, numerical modelling of OM-355 dual fuel (injection of diesel pilot fuel to premixed mixture of air and methane) engine has been performed by using KIVA-3V code at part and full loads. Sub-models of the code were modified to simulate the fuel spray atomization, combustion and pollutants emissions processes, accurately. Results indicate that in-cylinder pressure, heat release rate and exhaust emissions predictions are in good agreement with experiments at all loads. Results show that a lean premixed natural gas mixture is ignited slowly. The slow progress of combustion process at part load, leads the heat release to be drawn more toward the expansion stroke which causes incomplete combustion, and consequently high amounts of UHC and CO will be emitted. It is found that at part loads, areas that are influenced by diesel diffusion flames are ignited and premixed natural gas flame could not be propagated properly. Hence development of diesel diffusion flame is required to burn lean natural gas mixture. But at full load, in addition to the diesel diffusion flames, premixed natural gas flame could be propagated suitably. Also, at part load because of low gas temperature in the environment of diesel spray and low diesel fuel temperature, diesel liquid droplets evaporate lately which are far from injector nozzles. Hence, it causes diesel diffusion flame from spray of each injector nozzles to be developed distinctly. It can be deduced that the flame structure is affected by operating conditions. Finally the effect of increasing the diesel fuel quantity on improving methane combustion is studied. The studied strategy could help to improving natural gas combustion due to enlarge the size of diesel combustion region.

17/01978 An efficient auxiliary system controller for fuel cell electric vehicle (FCEV)

Lawrence, C. P. *et al. Energy*, 2016, 116, 417–428.

This article presents analysis of the systems in a fuel cell electric vehicle (FCEV) prototype with the aim of determining if it is possible to increase vehicle efficiency through strategic control of the auxiliary systems. To accomplish this, an overview of the vehicle design is given as well as an in depth analysis of the powertrain efficiency and control strategy. This leads to the development of a modified powertrain control algorithm which also oversees and controls the auxiliary power demand in real-time. The auxiliary control aspect of this algorithm follows predefined rules as determined through analysis of the individual systems, and based on the definitions of flexible useful and wasteful auxiliary power. The simulation results show that the proposed technique, applied to FCEV air conditioning system alone, improves the fuel economy in the neighbourhood of 3.4% compared to conventional bang-bang controller. This magnitude of energy reduction is very significant in the automotive industry, especially when considering the number of vehicles in use in today's transportation sector. The resulting algorithm is adaptable to a number of different types of auxiliary systems and primary power sources, thereby not specifically tied to the fuel cell architecture for which it is developed.

17/01979 ARIMA-based decoupled time series forecasting of electric vehicle charging demand for stochastic power system operation

Amini, M. H. *et al. Electric Power Systems Research*, 2016, 140, 378–390.

Large-scale utilization of electric vehicles (EVs) affects the total electricity demand considerably. Demand forecast is usually designed for the seasonally changing load patterns. However, with the high penetration of EVs, daily charging demand makes traditional forecasting methods less accurate. This paper presents an autoregressive integrated moving average (ARIMA) method for demand forecasting of conventional electrical load (CEL) and charging demand of EV (CDE) parking lots simultaneously. The EV charging demand prediction model takes daily driving patterns and distances as an input to determine the expected charging load profiles. The parameters of the ARIMA model are tuned so that the mean square error (MSE) of the forecaster is minimized. The accuracy of ARIMA forecaster was improved by optimizing the integrated and auto-regressive order parameters. Furthermore, due to the different seasonal and daily pattern of CEL and CDE, the proposed decoupled demand forecasting method provides significant improvement in terms of error reduction. The impact of EV charging demand on the accuracy of the proposed load forecaster is also analysed in two approaches: (1) integrated forecaster for CEL + CDE and (2) decoupled forecaster that targets CEL and CDE independently. The forecaster outputs are used to formulate a chance-constrained day-ahead scheduling problem. The numerical results show the effectiveness of the proposed forecaster and its influence on the stochastic power system operation.

17/01980 Combustion, gaseous and particulate emission of a diesel engine fueled with n-pentanol (C5 alcohol) blended with waste cooking oil biodiesel

Zhu, L. *et al. Applied Thermal Engineering*, 2016, 102, 73–79.

The combustion, gaseous and particulate emissions of a diesel engine fuelled with biodiesel–pentanol (BP) blends were investigated under different engine loads. The results indicate that with the increased pentanol fraction, the start of combustion is delayed. All of the BP blends provide faster combustion than biodiesel and diesel fuel from CA10 to CA90. The faster combustion of BP blends leads to a higher BTE than that of biodiesel and diesel fuel in most cases. The particle mass and number concentrations are reduced by the addition of pentanol in biodiesel in most test conditions, due to the higher oxygen concentration for the fuel/air stoichiometry, longer ignition delay for fuel/air mixing, and lower viscosity for the improvement of atomization. The R–(C=O)O–R′ group in biodiesel is less efficient in suppressing the soot precursor's formation than the R–OH group in pentanol. The diameter of the primary particles is reduced with the increased addition of pentanol. The particulate emission of BP10 have higher oxidation reactivity that that of BP20 and BP30. Base on this study, pentanol–biodiesel can be considered as an acceptable alternative fuel for diesel engines due to its improved combustion performance and reduced particulate emissions.

17/01981 Control design and fuel economy investigation of power split HEV with energy regeneration of suspension

Shi, D. *et al. Applied Energy*, 2016, 182, 576–589.

This paper explores the impacts of active suspension with energy regeneration capability on the fuel economy of a power split hybrid electric vehicle (HEV). Models of HEV powertrain and suspension are established and, based on their interactions, unified. The impacts of control parameters on the suspension performance are synthetically analysed. The analyses form a basis for the design of suspension controller. High-level supervisory controller and low-level sub-controllers for HEV powertrain and suspension are designed. Low-level sub-controllers can ensure the performance of each system, whose control parameters are updated by the supervisory controller. The equivalent consumption minimization strategy (ECMS), superior in maintaining charge sustainability, is improved for better application in the proposed system. Simulation results under different conditions demonstrate that both HEV fuel economy and ride comfort are improved. Comparative analyses of various scenarios validate the positive effect of suspension energy regeneration on the energy conservation performance of power split HEV. Meanwhile, the improvement of HEV fuel economy can be highlighted by applying ECMS.

17/01982 Difference in maximum torque-speed characteristics of induction machine between motor and generator operation modes for electric vehicle application

Guan, Y. *et al. Electric Power Systems Research*, 2016, 136, 406–414.

This paper explains the reason for the difference in maximum torque-speed characteristics and power factor of an induction machine (IM) between the motor and generator operation modes and investigates the influence of machine design parameters on the difference, such as stator resistance, rotor resistance and iron loss, etc. An analytical mathematical model based on the *dq* reference frame is employed for

investigation. It is shown that the difference in torque-speed characteristics between the motor and generator operation modes is mainly caused by the opposite direction of q-axis current and affected by stator and rotor resistance values. Finally, analytically calculated torque-speed characteristics of a 12 kW IM in the motor and generator operation modes are verified by finite element analyses.

17/01983 Economic assessment of phase reconfiguration to mitigate the unbalance due to plug-in electric vehicles charging

Gray, M. K. and Morsi, W. G. *Electric Power Systems Research*, 2016, 140, 329–336.

This paper investigates the economic feasibility of a phase reconfiguration approach to mitigate the unbalance impact of plug-in electric vehicles using split-phase level 1 charging on the secondary distribution system. The impact resulting from plug-in battery electric vehicles charging as single-phase loads in terms of reliability and power quality are quantified using a Monte Carlo Simulation. The cost-effectiveness of introducing phase reconfiguration in the secondary system is evaluated after mathematically formulating the phase reconfiguration as an optimization problem. The results have shown that the application of phase reconfiguration may result in a significant reduction in unbalance experienced by the system due to high penetration of plug-in battery electric vehicles taking into consideration the time of use pricing.

17/01984 Effect of ethanol fraction on the combustion and emission characteristics of a dimethyl ether-ethanol dual-fuel reactivity controlled compression ignition engine

Park, S. H. *et al. Applied Energy*, 2016, 182, 243–252.

The purpose of this study was to investigate the effect of the ethanol fraction on the combustion and exhaust emissions characteristics of dimethyl ether (DME)–ethanol dual-fuel reactivity controlled compression ignition (RCCI) engine. In this study, a modified single-cylinder diesel engine was used. The main parameters of this study were the in-cylinder injection timing of DME and the ethanol fraction. The ethanol fraction was found to have a more obvious effect on the indicated mean effective pressure (IMEP) for advanced in-cylinder injection timings than around the top dead centre (TDC) conditions. For the same ignition timing, the ethanol fraction had little influence on the IMEP. Increasing the ethanol fraction induced an increase in combustion duration and a decrease in premixed combustion duration (CA10–CA50) around the TDC injection condition. The effect of ethanol on P_{max} was insignificant for CA50. The application of the DME-ethanol dual-fuel combustion strategy caused a significant reduction of $ISNO_x$ without deterioration of ISsoot. In addition, a high ethanol fraction led to a low $ISNO_x$ for the same premixed combustion duration. The ISHC and ISCO emissions increased slightly with increasing ethanol fraction for DME–ethanol dual-fuel combustion. However, the emissions from DME–ethanol combustion were lower than those obtained previously with biodiesel–ethanol and diesel–ethanol dual-fuel combustion.

17/01985 Effects of pilot injection timing on the combustion noise and particle emissions of a diesel/natural gas dual-fuel engine at low load

Yang, B. *et al. Applied Thermal Engineering*, 2016, 102, 822–828.

For diesel pilot ignited dual-fuel engines, pilot injection timing is a very important parameter to control the initial combustion process. In this study, the combustion noise and particle emissions characteristics of a diesel/natural gas dual-fuel engine with varying pilot injection timing at low load (BMEP = 0.357 MPa) were experimentally investigated. The in-cylinder pressure, heat release rate (HRR), pressure raise rate (PRR), ignition delay, combustion duration and brake thermal efficiency (BTE), as well as THC, CO, NO_x and particle emissions were analysed. The maximum pressure rise rate was presented as a measure of combustion noise and the electrical low-pressure impactor (ELPI) was employed to illustrate the particle number and mass distributions. The experimental results indicated that the combustion noise is obviously deteriorated with advanced pilot injection timing. However, the particle number and mass concentrations could be reduced significantly with advanced pilot injection timing. In addition, the maximum reduction of particle number was more than 75%. Therefore, according to experimental study of combustion noise and particle emissions, it is not rational to excessively advance the pilot injection timing. Meanwhile the combustion noise can be considered as a limiting factor when advancing the pilot injection timing.

17/01986 Enabling dual fuel sequential combustion using port fuel injection of high reactivity fuel combined with direct injection of low reactivity fuels

Qian, Y. *et al. Applied Thermal Engineering*, 2016, 103, 399–410.

This paper presents a preliminary experimental study on the combustion and emission characteristics of dual fuel sequential combustion (DFSC) mode, in which port fuel injection of n-heptane combined with in-cylinder, directly injected ethanol, n-butanol and n-amyl alcohol are used in a single-cylinder engine at fixed directly injection timing. The results show that the heat release can be divided mainly into three stages: low temperature reaction, high temperature reaction of n-heptane and the directly injected fuel combustion stage. The amount of port injected n-heptane plays a key role in the maximum in-cylinder pressure (P_{max}), maximum in-cylinder mass averaged temperature (T_{max}) and the maximum pressure rise rate. For the high overall lower heating values (LHVs) per-cycle, the CO emissions decrease with the increase of the premixed ratio. By contrast, the CO emissions increase with the premixed ratio when the overall LHVs per-cycle are kept at medium and low levels. The NO_x and soot emissions are all kept at low levels for the experimental conditions. In particular, the higher latent heat, lower cetane values and the shorter carbon chains associated with ethanol lead to lower NO_x and soot emissions than those of n-butanol and n-amyl alcohol. When directly injection of n-butanol and at low loads, with optimized premixed ratio, the indicated thermal efficiency can be higher than 46% meanwhile maintaining low emissions.

17/01987 Enhancing the fuel economy and emissions performance of a gasoline engine-powered vehicle with idle elimination and hydrogen start

Ji, C. *et al. Applied Energy*, 2016, 182, 135–144.

Idle elimination is a feasible way for reducing the fuel consumption and emissions at idle. The challenge for adopting idle elimination on gasoline engine is the high emissions during restart because rich mixtures have to be used at starting. This paper tries to start the engine with pure hydrogen at the restart for gasoline vehicles which adopt idle elimination. The investigation was done based on models built on AVL CRUISE. In the model, the vehicle was run under the New European Driving Cycle (NEDC). The hydrogen used on the vehicle was online produced and stored by an on-board hydrogen production and storage system. The energy for producing hydrogen is taken into account in the total fuel consumption. The simulation results showed that, with the adoption of gasoline start-idle elimination strategy, the vehicle fuel consumption during NEDC was reduced by 0.69 L/100 km, and NO_x emissions were decreased by 5.5% compared with the original vehicle without idle elimination. However, HC and CO emissions at the restart were respectively increased by 87.5% and 18.1% for the gasoline vehicle due to the adoption of rich mixtures. Comparatively, with the adoption of hydrogen start-idle elimination strategy, the vehicle fuel consumption during NEDC was reduced by 0.79 L/100 km, HC and CO emissions were decreased by 70.8% and 13.6%, respectively. This shows a good capability of hydrogen combustion on reducing HC and CO emissions at the restart. However, NO_x emissions were slightly increased by 7.9% under the hydrogen restart mode.

17/01988 Gas/fuel jet interfaces under high pressures and temperatures

Falgout, Z. *et al. Fuel*, 2016, 168, 14–21.

This paper report observations regarding changes in surface morphology for transient fuel jets as the ambient conditions approach the critical properties of pure fuels. Both ballistic imaging and ultrafast shadow imaging were applied to four fuels as they were injected through a single hole diesel injector into a spray research chamber operated at three different ambient conditions that span the range of critical properties for the pure fuels that were studied. The results indicate that the pure fuels (butanol, dodecane, and hexadecane) tend to undergo a change in image structure that usually scales with estimated mixture critical properties. Commercially available diesel fuel is not strongly affected, even at the highest pressure and temperature conditions.

17/01989 Impact of control strategy on battery degradation for a plug-in hybrid electric city bus in China

Cai, Y. *et al. Energy*, 2016, 116, 1020–1030.

Series–parallel plug-in hybrid electric vehicles combine the advantages of series and parallel configurations and have been used in China. However, battery degradation in series-parallel plug-in hybrid electric city bus applications still needs to be investigated. In this paper, a simulation model is developed to simulate a series–parallel plug-in hybrid electric city bus. The simulation model was validated experimentally and shown to agree well with the real system. Additionally, a semi-empirical battery life model was also developed and validated to estimate the battery degradation. According to the simulation model and battery life model, the impact of different control strategies for series–parallel plug-in hybrid electric city buses on battery degradation was investigated. The simulation results showed that series–parallel plug-in hybrid electric city buses with the maximum efficiency control strategy for series mode and power follower control strategy for parallel mode reduced battery degradation significantly.

17/01990 Impact of pilot diesel ignition mode on combustion and emissions characteristics of a diesel/natural gas dual fuel heavy-duty engine

Wang, Z. *et al. Fuel*, 2016, 167, 248–256.

The brake thermal efficiency and exhaust emission issues are still not fully resolved to diesel/natural gas dual fuel engines. To better understand the effect of pilot diesel ignition mode on combustion and emissions characteristics of dual fuel engines, a detailed study concerned with diesel injection timing was conducted. The testing work was operated on a six-cylinder turbocharged intercooler diesel/natural gas dual fuel heavy-duty engine at light load operations, and diesel injection timing was controlled over a very wide range. The investigated results show that the diesel injection timing (T_{inj}) has an obvious effect on pilot diesel ignition mode. A significant advancing T_{inj} leads to pilot diesel ignition mode differs from traditional diesel engine compression ignition mode in the sense that it does not occur at a specific place in the spray, which is a two-stage autoignition mode. With advancing T_{inj}, engine combustion and emissions characteristics, including cylinder pressure, cylinder temperature, heat release rate, start of combustion (SOC), ignition delay, combustion duration, crank angle of 50% heat release (CA50), nitrogen oxides (NO_x) and total hydrocarbon (THC), show completely different variation trends in different ignition modes. Overall, higher thermal efficiency and lower emissions can be achieved simultaneously in two-stage autoignition mode. Satisfactory results can be obtained with higher brake thermal efficiency (35%), lower NO_x (60 ppm) and THC (0.4%) emissions, when T_{inj} is 42.5° CA BTDC.

17/01991 Influence of diesel fuel blended with biodiesel produced from waste cooking oil on diesel engine performance

Attia, A. M. A. *et al. Fuel*, 2016, 167, 316–328.

Biodiesel from edible waste cooking oil (waste cooking oil methyl ester – WCOME) has been produced via trans-esterification process. The effect of various fuel blends containing the conventional diesel fuel and the produced WCOME on diesel engine performance has been evaluated experimentally. The study investigated the effect of WCOME blending ratio on viscosity and sooting propensity of the biodiesel–diesel fuel mixture. The engine performance has been expressed in terms of the in-cylinder pressure data as well as the engine mechanical and environmental aspects measured at engine rated speed (1500 rpm) and different engine loads. The main results of the current work showed that, the location and value of the in-cylinder peak pressure depends mainly on the engine load and the biodiesel blending ratio. The best value of brake specific energy consumption (BSEC) is attained at blended fuel containing 20% WCOME (B20) where the maximum brake thermal efficiency is also observed. While there was a range of blending ratio from B20 to B50 throughout the best engine environmental behaviour is attained. Results indicated that, the use of neat biodiesel fuel (B100) at different engine loads leads to an increase of BSEC by about 8%, an increase of engine smoke opacity by about 15%, a decrease of NO_x emissions by about 10% with slight decrease of CO emissions and a decrease of the unburned hydrocarbons by about 15%. The most recommended WCOME biodiesel blending ratios vary from 30% to 50% for better engine performance and emission characteristics. In this recommended blending ratios, the engine performance provides the following results in comparison with the corresponding values for neat fuel around 10% higher BSFC, insignificant change in η_{bth}, around 3% higher BSEC, and 2% lower T_{Exh}, while the corresponding engine emissions include 25% lower CO, 20% lower UHC, 6% lower NO_x, and 20% higher smoke opacity.

17/01992 Influence of the heating system on the fuel consumption of a hybrid electric vehicle

Horrein, L. *et al. Energy Conversion and Management*, 2016, 129, 250–261.

This research work aims to study the impact of the heating system on the fuel consumption of a hybrid electric vehicle (HEV). The thermal engine is less used in an HEV than in a thermal vehicle, thus the cabin heating is partly ensured by electrical resistances. However, because the battery is partly charged by the thermal engine, this electrical heating has an impact on the fuel consumption. In the present work, a multi-domain model is proposed to analyse the impact of the heating system on the fuel consumption of a HEV. The models of the different physical subsystems are organized and unified by energetic macroscopic representation. Experimental validations, with an accuracy of 95%, are provided for each subsystem model. The validated simulation models are used to study the impact of the heating system for a specific driving cycle and climatic condition. For a simple energy management strategy (EMS), there is an over-consumption of 19% that is due to the heating system. When a more efficient EMS is used, the over-consumption is reduced to 12%. This study shows the interest in developing advanced energy management strategies that couple the traction and the heating functions of the vehicle.

17/01993 Model predictive control-based energy management strategy for a series hybrid electric tracked vehicle

Wang, H. *et al. Applied Energy*, 2016, 182, 105–114.

The series hybrid electric tracked bulldozer (HETB)'s fuel economy heavily depends on its energy management strategy. This paper presents a model predictive controller (MPC) to solve the energy management problem in an HETB for the first time. A real typical working condition of the HETB is utilized to develop the MPC. The results are compared to two other strategies: a rule-based strategy and a dynamic programming (DP) based one. The latter is a global optimization approach used as a benchmark. The effect of the MPC's parameters (e.g. length of prediction horizon) is also studied. The comparison results demonstrate that the proposed approach has approximately a 6% improvement in fuel economy over the rule-based one, and it can achieve over 98% of the fuel optimality of DP in typical working conditions. To show the advantage of the proposed MPC and its robustness under large disturbances, 40% white noise has been added to the typical working condition. Simulation results show that an 8% improvement in fuel economy is obtained by the proposed approach compared to the rule-based one.

17/01994 Modelling of evaporative losses in n-alcohol/diesel fuel blends

Hernández, J. P. *et al. Applied Thermal Engineering*, 2016, 102, 302–310.

Alcohol/diesel fuel blends allow reducing the formation of soot in diesel engines. However, its use in a large scale framework still faces the challenge of high evaporative losses under storage conditions which is hindered by the high volatility of the alcohols. Since the design of the most adequate fuelling system for each blend requires detailed knowledge about the evaporation losses from the liquid phase, in this work a method for calculating the evaporation of pure n-alcohols (from C1 to C5 carbon atoms) and blends of these alcohols with ultra-low sulfur diesel (ULSD) was proposed. Alcohols vapour pressure was determined with the Antoine equation, while the diffusion coefficient of alcohols in air was calculated as a function of carbon number and temperature. The coefficients of activity were obtained by the combination of continuous thermodynamic (gamma distribution function) and a modified UNIFAC-Dortmund-Continuous method. The evaporation losses model is based on Fick's law and exhibited good agreement with experimental data for all alcohols and blends at 20% content of all alcohols and at 20–60% contents of n-butanol with diesel fuel. The evaporation was found to decrease approximately with an inversely proportional rate with respect to the increase in the carbon chain length of the alcohol. The paradox of faster evaporative losses from blends with lower alcohol content is explained.

17/01995 Multi-agent based modeling for electric vehicle integration in a distribution network operation

Hu, J. *et al. Electric Power Systems Research*, 2016, 136, 341–351.

The purpose of this paper is to present a multi-agent based modelling technology for simulating and operating a hierarchical energy management of a power distribution system with a focus on electric vehicle (EV) integration. The proposed multi-agent system consists of four types of agents: (i) distribution system operator (DSO) technical agent and (ii) DSO market agents that both belong to the top layer of the hierarchy and their roles are to manage the distribution network by avoiding grid congestions and using congestion prices to coordinate the energy scheduled; (iii) EV virtual power plant agents are in the middle level of the hierarchy and their roles are to manage the charge process of the electric vehicles; (iv) EV agents are placed at the bottom layer of the hierarchy and they represent EV owners with different users' profiles. To demonstrate the coordination behaviour of the proposed system, a multi-agent simulation platform is developed based on the co-simulation environment of JACK, Matlab and GAMS. The aim of the multi-agent system is to simulate the collaborative (all agents contribute to achieve an optimized global performance) but also competitive environment (each agent will try to increase its utilities or reduce its costs).

17/01996 Multi-objective energy management optimization and parameter sizing for proton exchange membrane hybrid fuel cell vehicles

Hu, Z. *et al. Energy Conversion and Management*, 2016, 129, 108–121.

The powertrain system of a typical proton electrolyte membrane hybrid fuel cell vehicle contains a lithium battery package and a fuel cell stack. A multi-objective optimization for this powertrain system of a passenger car, taking account of fuel economy and system durability, is discussed in this paper. Based on an analysis of the optimum results obtained by dynamic programming, a soft-run strategy was proposed for real-time and multi-objective control algorithm design. The soft-run strategy was optimized by taking lithium battery size into consideration, and implemented using two real-time algorithms. When compared with the optimized dynamic programming results, the power demand-based

control method proved more suitable for powertrain systems equipped with larger capacity batteries, while the state of charge based control method proved superior in other cases. On this basis, the life cycle cost was optimized by considering both lithium battery size and equivalent hydrogen consumption. The battery capacity selection proved more flexible, when powertrain systems are equipped with larger capacity batteries. Finally, the algorithm has been validated in a fuel cell city bus. It gets a good balance of fuel economy and system durability in a three months demonstration operation.

17/01997 Nonlinear autoregressive neural network in an energy management strategy for battery/ultra-capacitor hybrid electrical vehicles
Ibrahim, M. *et al. Electric Power Systems Research*, 2016, 136, 262–269.
Hybrid electric vehicles are one of the most promising solutions for reducing pollution and fuel consumption. However, their propulsion system comprises a number of different on-board power sources with different dynamic characteristics, meaning that some strategy is required for sharing power between them that takes their characteristics into account. In this paper, a new real time energy management strategy for battery/ultra-capacitor hybrid vehicles is proposed. This strategy is based on sharing the total power between the on-board power systems, namely the battery and the ultra-capacitors, using a non-linear auto-regressive neural network as a time series prediction model and discrete wavelet transform as a time-frequency filter. The objective of this strategy is to lengthen the life of the battery. This new strategy was simulated using actual data from a military hybrid vehicle. The results were found to be promising and show the robustness of the proposed method.

17/01998 Performance and combustion characteristics of a diesel engine fuelled by butanol–biodiesel–diesel blends
Ibrahim, A. *Applied Thermal Engineering*, 2016, 103, 651–659.
Using renewable alternative fuels in the diesel engines has been grown recently. The aim of the study was to experimentally investigate and compare the performance, combustion characteristics, NO emissions, and stability of a diesel engine fuelled by five different fuels, which included diesel, biodiesel, and different blends of diesel–biodiesel–butanol mixtures. All the tests were conducted using a single-cylinder direct-injection diesel engine at a speed of 1500 rpm and different engine load conditions. It was found that the optimum alternative fuel among all the tested fuels was the B50 fuel blend as its use increased the maximum engine thermal efficiency by 6.5% and decreased the lowest engine brake specific fuel consumption by 5% compared to the diesel fuel. NO emission increased significantly with increasing the engine load and increased slightly with using oxygenated fuels. The change of fuel type had no significant effect on the combustion start timing while the combustion duration increased with increasing the engine load. All the tested fuels did no negatively affect the engine stability.

17/01999 Risk management and participation planning of electric vehicles in smart grids for demand response
Nezamoddini, N. and Wang, Y. *Energy*, 2016, 116, 836–850.
Demand response (DR) can serve as an effective tool to better balance the electricity demand and supply in the smart grid. It is defined as 'the changes in electricity usage by end-use customers from their normal consumption patterns' in response to pricing and incentive payments. This paper focuses on new opportunities for DR with electric vehicles (EVs). EVs are potential distributed energy resources that support both the grid-to-vehicle and vehicle-to-grid modes. Their participation in the time-based (e.g. time-of-use) and incentive-based (e.g. regulation services) DR programmes helps improve the stability and reduce the potential risks to the grid. Smart scheduling of EV charging and discharging activities also supports high penetration of renewables with volatile energy generation. This paper proposes a novel stochastic model from the independent system operator's perspective for risk management and participation planning of EVs in the smart grid for DR. The risk factors considered in this paper involve those caused by uncertainties in renewables (wind and solar), load patterns, parking patterns, and transmission lines' reliability. The effectiveness of the model in response to various settings such as the area type (residential, commercial, and industrial), the EV penetration level, and the risk level has been investigated.

17/02000 Simulated annealing to handle energy and ancillary services joint management considering electric vehicles
Sousa, T. *et al. Electric Power Systems Research*, 2016, 136, 383–397.
The massive use of distributed generation and electric vehicles will lead to a more complex management of the power system, requiring new approaches to be used in the optimal resource scheduling field. Electric vehicles with vehicle-to-grid capability can be useful for the aggregator players in the mitigation of renewable sources intermittency and in the ancillary services procurement. In this paper, an energy and ancillary services joint management model is proposed. A simulated annealing approach is used to solve the joint management for the following day, considering the minimization of the aggregator total operation costs. The case study considers a distribution network with 33-bus, 66 distributed generation and 2000 electric vehicles. The proposed simulated annealing is matched with a deterministic approach allowing an effective and efficient comparison. The simulated annealing presents a solution closer to the one obtained in the deterministic approach (1.03% error), yet representing 0.06% of the deterministic approach CPU time performance.

Transport battery development

17/02001 A comprehensive review of on-board state-of-available-power prediction techniques for lithium-ion batteries in electric vehicles
Farmann, A. and Sauer, D. U. *Journal of Power Sources*, 2016, 329, 123–137.
This study provides an overview of available techniques for on-board state-of-available-power (SoAP) prediction of lithium-ion batteries (LIBs) in electric vehicles. Different approaches dealing with the on-board estimation of battery state-of-charge (SoC) or state-of-health (SoH) have been extensively discussed in various researches in the past. However, the topic of SoAP prediction has not been explored comprehensively yet. The prediction of the maximum power that can be applied to the battery by discharging or charging it during acceleration, regenerative braking and gradient climbing is definitely one of the most challenging tasks of battery management systems. In large lithium-ion battery packs because of many factors, such as temperature distribution, cell-to-cell deviations regarding the actual battery impedance or capacity either in initial or aged state, the use of efficient and reliable methods for battery state estimation is required. The available battery power is limited by the safe operating area (SOA), where SOA is defined by battery temperature, current, voltage and SoC. Accurate SoAP prediction allows the energy management system to regulate the power flow of the vehicle more precisely and optimize battery performance and improve its lifetime accordingly. To this end, scientific and technical literature sources are studied and available approaches are reviewed.

17/02002 A honeycomb-cobweb inspired hierarchical core–shell structure design for electrospun silicon/carbon fibers as lithium-ion battery anodes
Wu, J. *et al. Carbon*, 2016, 98, 582–591.
The silicon/carbon (Si/C) hybrid fibres with a hierarchical core–shell structure are prepared by encapsulating Si nanoparticles in the interconnected hollow carbon fibres (Si@IHCFs) based on a dual coaxial electrospinning technique. For the hierarchical structure, Si nanoparticles are embedded in the honeycomb-like carbon framework in the fibre core, which is further wrapped by the interlocked cobweb-like carbon shell network. As lithium-ion battery anode, the well-defined Si@IHCFs demonstrates a reversible capacity of 903 mAh g^{-1} and a capacity retention of 89% after 100 cycles with a current density of 0.2 A g^{-1}. With the current density gradually increasing to 2.0 A g^{-1}, the electrode shows a specific capacity of 743 mAh g^{-1}, exhibiting superior rate capability compared to the Si/C fibres with a core–shell but unconnected structure. The excellent electrochemical properties are attributed to the hierarchical core–shell structure and cross-linked network for the Si/C composite fibres. The carbon framework in the core region accommodates the volume expansion of Si by the honeycomb-like pores. And the interconnected carbon shell can not only prevent electrolyte from permeating into the core section, but also improve the electronic conductivity by the connections in the fibre network.

17/02003 A novel ultrasonic velocity sensing approach to monitoring state of charge of vanadium redox flow battery
Chou, Y.-S. *et al. Applied Energy*, 2016, 182, 253–259.
A novel ultrasonic velocity sensing approach is proposed and investigated to monitor the state of charge (SOC) of a vanadium redox flow battery (VRB). The positive electrode is designated as the energy storage capacity-limiting one so that the molar ratio of the V^{5+} ion in the positive electrolyte solution determines the SOC of a VRB. The tested single-cell VRB is connected to an ultrasonic sensor and charged/discharged almost to its two extremes at a constant current of 2 A under various operating temperatures. It is found that the ultrasound velocity exhibits distinct variations in accordance with changes of vanadium ion compositions in the positive electrolyte solution as the SOC of the VRB varies. The SOC obtained can be depicted in a 3D plot in terms of ultrasound velocity and operating temperature. An empirical model equation is proposed and found to fit

the experimental results of both charging and discharging stages quite well. The advantages of this SOC sensing approach are that it is totally independent of VRB operations and can be readily applied to both sides of the electrodes. It is expected to develop into a dependable method for accurate and real-time monitoring of SOC for VRB.

17/02004 A probability load modeling method for the charging demand of large-scale PEVs accounting users' charging willingness

Xu, H. *et al. International Journal of Electrical Power & Energy Systems*, 2016, 82, 331–338.

This paper presents a new strategy in order to model the charging power demand due to large-scale plug-in electric vehicles (PEVs) as realistic a fashion as possible and analyse their impact on the residential power distribution system. The strategy takes the charging willingness of PEV users into consideration, and accounts for the difference in charging frequencies among users. A detailed classification, derived from the historical data on users' driving patterns, on PEV users is conducted in order to ensure that users in the same user set have the same charging properties. Seven probability load models for PEV charging are established for these user sets, and each model accounts the inherent randomness in the usages and recharges of PEVs. After the consideration of charging willingness, the charging demand differs among weekdays. The aggregated charging demand from a user set on each weekday is calculated based on the Law of Large Numbers, and the total charging demand from all PEVs on each weekday can be obtained by accumulating the aggregated charging demand of the user sets with charging willingness. The strategy can ensure a high utilization of the battery capacity, and the aggregated charging demand resulted is more rational and credible. The proposed charging load modelling strategy is finally applied on the electric load profile on a winter day in Manitoba.

17/02005 A promising cathode for Li-ion batteries: $Li_3V_2(PO_4)_3$

Liu, C. *et al. Energy Storage Materials*, 2016, 4, 15–58.

Lithium ion batteries are essential energy storage devices that power the electronics that let us share information and connect with people anywhere at any time. As the demand for uninterrupted energy performance rises, corresponding challenges need to be overcome in both industry and academia. Currently, cathode performance limits energy-power density in Li-ion batteries. Materials chemists and scientists have devoted much effort to explore cathodes with higher capacities and electrochemical potentials. Lithium vanadium phosphate, a rising star in the cathode family, has attracted more attention in recent years because it can display a high average potential (>4.0 V) and specific capacity (197 mAh/g) with excellent structural stability during cycling. However, the separated VO_6 octahedra intrinsically limit electrical conductivity, which hurts the rate capability. This review focuses on the fundamental issues in lithium vanadium phosphate and summarizes its crystal structure, ion diffusion, and electrochemical characteristics. Three synthetic aspects are described carefully: doping, composite and designing microstructures. At the same time, some rules are distilled from the report results, which may be referred to in order to tune the electrochemical performance in electrode materials.

17/02006 A simplified multi-particle model for lithium ion batteries via a predictor-corrector strategy and quasi-linearization

Li, X. *et al. Energy*, 2016, 116, 154–169.

The design of a simplified yet accurate physics-based battery model enables researchers to accelerate the processes of the battery design, aging analysis and remaining useful life prediction. In order to reduce the computational complexity of the pseudo two-dimensional mathematical model without sacrificing the accuracy, this paper proposes a simplified multi-particle model via a predictor–corrector strategy and quasi-linearization. In this model, a predictor–corrector strategy is used for updating two internal states, especially used for solving the electrolyte concentration approximation to reduce the computational complexity and reserve a high accuracy of the approximation. Quasi-linearization is applied to the approximations of the Butler–Volmer kinetics equation and the pore wall flux distribution to predict the non-uniform electrochemical reaction effects without using any non-linear iterative solver. Simulation and experimental results show that the isothermal model and the model coupled with thermal behaviour are greatly improve the computational efficiency with almost no loss of accuracy.

17/02007 Butler-Volmer equation-based model and its implementation on state of power prediction of high-power lithium titanate batteries considering temperature effects

Jiang, J. *et al. Energy*, 2016, 117, 58–72.

This paper provides a further step towards popularizing the proposed Butler–Volmer (BV) equation-based model and its implementation on state of power (SOP) prediction at various temperatures, which is based on the relationship between state of charge and state of useful charge. The actual 10 s SOP of battery is obtained using the constant current pulse when the restriction of voltage is exactly managed. The COMPLEX method is taken to determine the coefficients of the simplified form of BV equation, enabling online estimation of battery states. Robustness analysis of the proposed model and algorithm on SOP prediction over a large temperature range is analysed and verified, showing their reliability and accuracy in estimating the terminal voltage and predicting power capability.

17/02008 Capacity fade modelling of lithium-ion battery under cyclic loading conditions

Ashwin, T. R. *et al. Journal of Power Sources*, 2016, 328, 586–598.

A pseudo two-dimensional (P2D) electro-chemical lithium-ion battery model is presented in this paper to study the capacity fade under cyclic charge-discharge conditions. The Newman model has been modified to include a continuous solvent reduction reaction responsible for the capacity fade and power fade. The temperature variation inside the cell is accurately predicted using a distributed thermal model coupled with the internal chemical heat generation. The model is further improved by linking the porosity variation with the electrolyte partial molar concentration, thereby proving a stronger coupling between the battery performance and the chemical properties of electrolyte. The solid electrolyte interface (SEI) layer growth is estimated for different cut-off voltages and charging current rates. The results show that the convective heat transfer coefficient as well as the porosity variation influences the SEI layer growth and the battery life significantly. The choice of an electrolyte decides the conductivity and partial molar concentration, which is found to have a strong influence on the capacity fade of the battery. The present battery model integrates all essential electro-chemical processes inside a lithium-ion battery under a strong implicit algorithm, proving a useful tool for computationally fast battery monitoring system.

17/02009 Capillary suspensions as beneficial formulation concept for high energy density Li-ion battery electrodes

Bitsch, B. *et al. Journal of Power Sources*, 2016, 328, 114–123.

This paper introduces a novel formulation concept to prepare high capacity graphite electrodes for lithium ion batteries. The concept is based on the capillary suspension phenomenon: graphite and conductive agent are dispersed in an aqueous binder solution and the organic solvent octanol is added as immiscible, secondary fluid providing the formation of a sample-spanning network resulting in unique stability and coating properties. No additional processing steps compared to conventional slurry preparation are required. The resulting ultra-thick electrodes comprise mass loadings of about 16.5 mg cm^{-2}, uniform layer thickness, and superior edge contours. The adjustment of mechanical energy input ensures uniform distribution of the conductive agent and sufficient electronic conductivity of the final dry composite electrode. The resulting pore structure is due to the stable network provided by the secondary fluid, which evaporates residue-free during drying. Constant current–constant potential (CC–CP) cycling clearly indicates that the corresponding microstructure significantly improves the kinetics of reversible Li^+ (de-)intercalation. A double layer electrode combining a conventionally prepared layer coated directly onto the Cu current collector with an upper layer stabilized with octanol was prepared applying wet-on-wet coating. CC–CP cycling data confirms that staged porosity within the electrode cross-section results in superior electrochemical performance.

17/02010 Effect of extreme temperatures on battery charging and performance of electric vehicles

Lindgren, J. and Lund, P. D. *Journal of Power Sources*, 2016, 328, 37–45.

Extreme temperatures pose several limitations to electric vehicle (EV) performance and charging. To investigate these effects, the authors combine a hybrid artificial neural network-empirical Li-ion battery model with a lumped capacitance EV thermal model to study how temperature will affect the performance of an EV fleet. It was found that at −10 °C, the self-weighted mean battery charging power (SWMCP) decreases by 15% compared to standard 20 °C temperature. Active battery thermal management (BTM) during parking can improve SWMCP for individual vehicles, especially if vehicles are charged both at home and at workplace; the median SWMCP is increased by over 30%. Efficiency (km/kWh) of the vehicle fleet is maximized when ambient temperature is close to 20 °C. At low (−10 °C) and high (+40 °C) ambient temperatures, cabin preconditioning and BTM during parking can improve the median efficiency by 8% and 9%, respectively. At −10 °C, preconditioning and BTM during parking can also improve the fleet SOC by 3–6%-units, but this also introduces a 'base' load of around 140 W per vehicle. Finally, it was observed that the utility of the fleet can be increased by 5%-units by adding 3.6 kW chargers to workplaces, but further improved charging infrastructure would bring little additional benefit.

17/02011 Effects of moist air on the cycling performance of non-aqueous lithium-air batteries

Tan, P. *et al. Applied Energy*, 2016, 182, 569–575.

Most non-aqueous lithium-air batteries reported in the literature are limited to operating with pure oxygen. To practically operate the battery in ambient air, understanding how the battery's performance varies with humidity of moist air is essential. This study considers the effects of moist air on the cycling performance through operating a non-aqueous lithium-air battery with a stable anode and a nano-structured RuO_2/NiO cathode at various relative humidities. Results show that in the dry air, the discharge and charge terminal voltages are around 2.51 and 4.12 V, respectively, but change to 2.79 and 3.87 V when the relative humidity reaches 84%. The energy efficiencies corresponding to the dry air and the relative humidity of 84% are 66.2% and 73.8%, respectively. The improved performance is found to be mainly due to the increased fraction of LiOH among the discharge products at high relative humidities. The discharge voltage for the formation of LiOH is higher than that for the formation of Li_2O_2, while the charge voltage for the decomposition of LiOH is lower than that for the decomposition of Li_2O_2. The results suggest that to enable a non-aqueous lithium-air battery to operate in moist air, in addition to protecting the lithium anode from water, designing a cathode with electrocatalytic activities for the decomposition of both Li_2O_2 and LiOH is required.

17/02012 Emerging non-lithium ion batteries

Wang, Y. *et al. Energy Storage Materials*, 2016, 4, 103–129.

Lithium ion batteries have dominated the field of electrochemical energy storage for the last 20 years. It still remains to be one of the most active research fields. However, there are difficult problems still surrounding lithium ion batteries, such as high cost, unsustainable lithium resource and safety issues. Rechargeable batteries base on alternative metal elements (Na, K, Mg, Ca, Zn, Al, etc.) can provide relatively high power density and energy density using abundant, low-cost materials. Therefore, non-lithium ion batteries are regarded as promising candidates to partially replace lithium ion batteries in near future. In recent years, the research on non-lithium rechargeable batteries is progressing rapidly, but many fundamental and technological obstacles remain to be overcome. Here the authors provide an overview of the current state of non-lithium rechargeable batteries based on monovalent metal ions (Na^+ and K^+) and multivalent metal ions (Mg^{2+}, Ca^{2+}, Zn^{2+} and Al^{3+}). The needs and possible choices of superior electrode materials and compatible electrolytes beneficial for ion transport were emphatically discussed in this review.

17/02013 Energy advancement integrated predictive optimization of photovoltaic assisted battery energy storage system for cost optimization

Syed, I. M. and Raahemifar, K. *Electric Power Systems Research*, 2016, 140, 917–924.

This paper presents a forecast-based predictive optimization for a grid-tied photovoltaic integrated battery energy storage system to minimize consumption from the grid. Forecasts of load demand and photovoltaic with tariff structure and battery energy storage system status are used as decision variables. Forecast-based predictive optimization with battery energy storage system control (energy usage advancement) increases photovoltaic proportion, decreases consumption from the grid during high price periods and reduces cost based on the present and futuristic load demand and photovoltaic potential. The proposed scheme allows consumers to manage their energy consumption, and thus cost, in response to energy price variation (time-of-use tariff) throughout the day by optimizing energy usage in high price periods. The proposed scheme is simple, effective, realistic, and accounts for errors in the forecasts. Results show noticeable savings in energy cost for a consumer and increased usage of otherwise wasted photovoltaic energy.

17/02014 Episodic air quality impacts of plug-in electric vehicles

Razeghi, G. *et al. Atmospheric Environment*, 2016, 137, 90–100.

In this paper, the spatially and temporally resolved energy and environment tool (STREET) is used in conjunction with University of California Irvine – California Institute of Technology (UCI-CIT) atmospheric chemistry and transport model to assess the impact of deploying plug-in electric vehicles and integrating wind energy into the electricity grid on urban air quality. STREET is used to generate emissions profiles associated with transportation and power generation sectors for different future cases. These profiles are then used as inputs to UCI-CIT to assess the impact of each case on urban air quality. The results show an overall improvement in 8-h averaged ozone and 24-h averaged particulate matter concentrations in the south coast air basin with localized increases in some cases. The most significant reductions occur north-east of the region where baseline concentrations are highest (up to 6 ppb decrease in 8-h-averaged ozone and 6 $\mu g/m^3$ decrease in 24-h-averaged $PM_{2.5}$). The results also indicate that, without integration of wind energy into the electricity grid, the temporal vehicle charging profile has very little to no effect on urban air quality. With the addition of wind energy to the grid mix, improvement in air quality is observed while charging at off-peak hours compared to the business as usual scenario.

17/02015 Monodispersed SnO_2 nanospheres embedded in framework of graphene and porous carbon as anode for lithium ion batteries

Miao, C. *et al. Energy Storage Materials*, 2016, 3, 98–105.

Tin peroxide (SnO_2) is one of most potential anode materials for lithium ion batteries with high energy density because of its appropriate (de)lithiation potential and high specific capacity. However, the poor cycling property of SnO_2 restricts its wide application in lithium ion battery. Herein, a novel monodispersed porous SnO_2 nanospheres/graphene/porous carbon composite electrode with excellent performance is constructed. In this electrode, the SnO_2 nanospheres with a diameter of ~60 nm are embedded in porous carbon, which is filled between the interlayers of graphene sheets. The carbon can protect the SnO_2 nanospheres from contacting with the electrolyte. The pores inside both SnO_2 nanospheres and carbon can accommodate the huge volume expansion of SnO_2 nanoparticles during charge–discharge process. The graphene sheets can greatly improve the strength, stability and flexibility of the electrode. The framework formed by graphene and porous carbon can successfully prevent the aggregation of SnO_2 nanospheres and collapse of SnO_2 composite electrode. As a result, the composite electrode shows excellent rate performance, which achieves discharge capacities of 816.3, 704.6, 600 and 459.4 mAh g^{-1} at current densities of 0.2, 0.5, 1 and 2 A g^{-1} and delivers a capacity of 873.2 mAh g^{-1} after 200 cycles at 0.2 A g^{-1}.

17/02016 Nanocellulose-laden composite polymer electrolytes for high performing lithium–sulphur batteries

Nair, J. R. *et al. Energy Storage Materials*, 2016, 3, 69–76.

In the endless search for superior and green power sources, lithium sulfur (Li–S) batteries held the promise of opening up a new era of long lasting and high energy storage systems for variety of applications. They might envisage remarkable benefits in utilizing polymer electrolytes instead of liquids in terms of safety, low-cost and gravimetric/volumetric energy densities. In this work, for the first time, nanoscale microfibrillated cellulose-laden polymer systems are prepared using a thermally induced polymerization process and tested as electrolyte separator in a Li–S rechargeable battery that contains sulfur–carbon composite based cathode. The polymer electrolyte demonstrates excellent ionic conductivity, thermal stability and most importantly stable interface towards lithium metal. While comparing the earlier report with non-aqueous liquid electrolyte, the present cell based on the abundant truly-natural cellulose-based polymer electrolyte as separator exhibits better cycling stability, higher specific capacity, superior Coulombic efficiency and rate capability at ambient conditions.

17/02017 $Na_{0.282}V_2O_5$: a high-performance cathode material for rechargeable lithium batteries and sodium batteries

Cai, Y. *et al. Journal of Power Sources*, 2016, 328, 241–249.

$Na_{0.282}V_2O_5$ nanorods have been successfully prepared using a facile hydrothermal reaction followed by a calcination treatment, which is then used as a cathode for lithium batteries and sodium batteries for the first time. The crystal structure is refined to be a monoclinic lattice, which contains 3D tunnels along the *b*-axis. The Na ions are located inside the tunnels and form 'pillar effect' to prevent the collapse of the crystal structure. As cathode material for lithium batteries, the $Na_{0.282}V_2O_5$ nanorods deliver a high discharge specific capacity of 264, 186, 191 and 149 mA h g^{-1} at the current density of 50, 500, 1000 and 1500 mA g^{-1}, respectively. The $Na_{0.282}V_2O_5$ nanorods demonstrate the excellent cycling performance up to 400 cycles at 1 and 1.5 A g^{-1}. Importantly, as cathode material for sodium batteries, $Na_{0.282}V_2O_5$ exhibits superior long-term cyclic stability up to 1000 cycles at 0.3 A g^{-1}. The results of *ex situ* XRD, EIS and first-principle calculation indicate that the $Na_{0.282}V_2O_5$ possesses good electrical conductivity and structural stability. This work demonstrates that the $Na_{0.282}V_2O_5$ material could be considered as a potential cathode for lithium-ion batteries, and even sodium ion batteries.

17/02018 Poly(*m*-phenylene isophthalamide) separator for improving the heat resistance and power density of lithium-ion batteries

Zhang, H. *et al. Journal of Power Sources*, 2016, 329, 8–16.

A microporous poly(*m*-phenylene isophthalamide) (PMIA) separator with high safety (high-heat resistance and self-extinguishing), high porosity and excellent liquid electrolyte wettability was prepared by the traditional non-solvent introduced phase separation process. Due to the high-heat resistance of PMIA material, the as-prepared separator exhibited a negligible thermal shrank ratio at 160 °C for 1 h. Meanwhile, benefiting from its high porosity and excellent wettability in liquid electrolyte, the liquid electrolyte uptake and the ionic

conductivity of the separator were higher than that of the commercial PP-based separators. Furthermore, the cell assembled with this separator showed better cycling performance and superior rate capacity compared to those with PP-based separators. These results suggested that the PMIA separator is very attractive for high-heat resistance and high-power density lithium-ion batteries.

17/02019 Resonant inductive power transfer for an E-bike charging station

Iannuzzi, D. *et al. Electric Power Systems Research*, 2016, 140, 631–642.

This paper presents the design and the experimental tests of an E-bike 300-W battery charger for a cyclo-station based on wireless power technology. In particular, a series resonant inductive power converter with an E-geometry magnetic core topology is proposed. A mathematical model is developed and a performance analysis is conducted to determine the voltage transfer function, maximum power transfer capability, efficiency for different air-gaps (1–3 cm) and misalignments (0.5–1.5 cm). Also, it is performed analytical and experimental investigations of the minimum and maximum relative frequency points of active input power and efficiency in order to determine how these points changed as the resistance load varied. The results of the analyses indicated that the maximum frequency points of active input power are different from the maximum frequency points of efficiency and the zero-frequency points of reactive input power. This means that maximum power transfer and efficiency conversion are not obtained in correspondence with the resonant frequency. For this purpose, it is conducted a wide frequency characterization of 30–50 kHz around the designed resonant frequency of 40 kHz. An iterative electrical and magnetic design procedure is proposed based on 3D finite element analysis. Simulation and experimental results are presented for a full-sized prototype. The design of the E-bike battery charger is validated in terms of rated input voltage and output power for different air-gap configurations.

17/02020 Sizing standalone battery charging systems based on photovoltaic (PVTCP) temperature crossing points using voltage source photovoltaic model (VSPVM)

Kibirige, B. *Solar Energy*, 2016, 136, 342–348.

Rural and semi-rural communities in developing countries harness solar energy mostly by using standalone photovoltaic (PV) battery charging systems. Basic electronics circuits that do not include direct current to direct current (DC–DC) voltage converters are employed. These provide raw voltage levels from the solar PV modules that sometimes charge batteries insufficiently, leading to shorter battery lives. By modelling the solar PV module using a voltage source circuit representation, the effects of temperature on the PV module voltage could easily be illustrated to these rudimentary trained communities that deal mostly with voltage sources and not current sources. A voltage source PV model (VSPVM) was developed from the well understood PV cell mathematical model. Microsoft Excel was used as the data fitting environment and the PSpice environment was used to capture the electronic circuit topology proposed for the VSPVM. Validating the model against experimental data fitted maximum power points within 5% of the experimental data. Observations made on *I–V* characteristics plotted on the same graph showed interesting patterns of crossing points referred to here as photovoltaic temperature crossing points. A low temperature cluster and a high temperature cluster which were indicative of thresholds of some sort were observed. For hot climate regions, the power point voltage which exists between the two clusters could be considered as a guide to the possible range within which a PV battery charging system should operation.

17/02021 State-of-health estimation of lithium-ion battery packs in electric vehicles based on genetic resampling particle filter

Bi, J. *et al. Applied Energy*, 2016, 182, 558–568.

Power battery packs are the energy source of battery electric vehicles (BEVs). A precise state-of-health (SOH) estimation for batteries is crucial to ensure the operational security and stability of BEVs. This paper employs an equivalent circuit model of battery pack in SOH estimation. Since a battery pack is a complex and non-linear system, the equivalent circuit model of battery pack is always complicated. To balance estimation accuracy and computational complexity, the equivalent circuit model of battery pack should be simplified. However, much noise is produced in the simplified model. In addition, the errors during SOH estimation are from various sources so that SOH estimation is a non-Gaussian problem. Given the genetic resampling particle filter (GPF) performs efficiently in solving non-Gaussian problems, this paper proposes a new GPF-based method for battery SOH dynamic estimation when accuracy of the equivalent circuit model is not high. First, a second-order equivalent circuit model of resistance–capacitance (RC) circuit for the battery pack is developed. The unknown parameters are identified using the recursive least-squares method with forgetting factor. Second, a state-space model of the GPF is developed based on the equivalent circuit model. Finally, a case study is conducted using real data collected from operating electric taxis in Beijing to investigate the estimation performance of the proposed model. Estimation results show that the proposed GPF model outperforms the particle filter method in the SOH estimation problem.

17/02022 Surface modification of over-lithiated layered oxide by low-temperature chemical vapor deposition for high energy lithium-ion batteries

Son, I. H. *et al. Energy Storage Materials*, 2016, 4, 137–144.

In comparison to traditional lithium ion battery cathode materials, over-lithiated layered oxides cathodes (OLOs) contain extra lithium ions. Because of this over-lithiation, they are considered a promising candidate for application as the cathode material in high-energy lithium ion batteries. However, to utilize the additional lithium ions, OLOs must be charged beyond 4.4 V vs Li/Li^+, i.e. highly oxidizing conditions. Consequently, oxidative side reactions on the surface of OLOs are problematic, hindering the performances of these lithium ion batteries. To overcome this problem, the authors developed an artificial homogeneous solid electrolyte interface (a-SEI) comprising an organic surface coating on OLO. The surface coating is deposited by low temperature-chemical vapour deposition using a mix of CO_2 and CH_4 gases. Using X-ray photoelectron spectroscopy and Fourier transform infrared spectroscopy, it was determined that the modified a-SEI is composed of alkylcarbonate and lithium carbonate. The surface modified OLO shows improved performance due to its enhanced rate capability, high initial capacity, and long cycle life. The authors used AC impedance analyses to investigate these improvements and found that they result from fast charge transfer reactions and the stabilization of the surface via surface modification.

17/02023 Technical and economic assessment of the secondary use of repurposed electric vehicle batteries in the residential sector to support solar energy

Assunção, A. *et al. Applied Energy*, 2016, 181, 120–131.

Photovoltaic (PV) generation, due to its decreasing cost and versatility, has seen a growing utilization in residential buildings. However, the mismatch between the demand and the PV generation profiles leads to high power flows between households and the grid. The appearance of tariffs that foster the self-consumption and penalize the injection of energy into the electrical grid increases the need to provide cost-effective solutions to enable the matching between electric generation and consumption. Used electric vehicle (EV) batteries are unsuitable for vehicles, but can be used in secondary applications, such as residential PV energy storage. This paper presents a technical and economic assessment of the reuse of batteries from electric vehicles as a storage system for the residential sector by analysing the cost, the remaining capacity and the lifetime for second applications through the implementation of a degradation model in MATLAB-Simulink. A case study is presented for an average southern Europe residential building with a photovoltaic system that generates enough energy to ensure the average consumption needs.

17/02024 The correlation of the properties of pyrrolidinium-based ionic liquid electrolytes with the discharge–charge performances of rechargeable Li–O_2 batteries

Li, Y. *et al. Journal of Power Sources*, 2016, 329, 207–215.

Pyrrolidinium-based ionic liquids (ILs), such as $PYR_{13}TFSI$, $PYR_{14}TFSI$, and $PYR_{1(2O1)}TFSI$, exhibit high thermal and electrochemical stability with wide electrochemical windows as electrolytes for application to rechargeable Li–O_2 batteries. In this work, several fundamental properties of three ILs are measured: the ionic conductivity, oxygen solubility, and oxygen diffusion coefficient. The oxygen electro-reduction kinetics is characterized using cyclic voltammetry. The performances of Li–O_2 batteries with these IL electrolytes are also investigated using electrochemical impedance spectroscopy and galvanostatic discharge–charge tests. The results demonstrate that the $PYR_{1(2O1)}$ TFSI electrolyte battery has a higher first-discharge voltage than the $PYR_{13}TFSI$ electrolyte and $PYR_{14}TFSI$ electrolyte batteries. Both $PYR_{13}TFSI$- and $PYR_{1(2O1)}TFSI$-based batteries exhibit higher first-discharge capacities and better cycling stabilities than the $PYR_{14}TFSI$-based battery for 30 cycles. A theoretical analysis of the experimental results shows that the diffusion coefficient and solubility of oxygen in the electrolyte remarkably affect the discharge capacity and cycling stability of the batteries. Particularly, the oxygen diffusion coefficient of the IL electrolyte can effectively facilitate the electrochemical oxygen electro-reduction reaction and oxygen concentration distribution in the catalyst layers of air electrodes. The oxygen diffusion coefficient and oxygen solubility improvements of IL electrolytes can enhance the discharge–charge performances of Li–O_2 batteries.

17/02025 The effects of design parameters on the charge-discharge performance of iron-chromium redox flow batteries
Zeng, Y. K. *et al. Applied Energy*, 2016, 182, 204–209.
The objective of this work is to understand and identify key design parameters that influence the battery performance of iron-chromium redox flow batteries (ICRFBs). The investigated parameters include the membrane thickness, electrode compression ratio, electrode pretreatment and catalyst loading. Results show that: (i) with a thin NR-211 membrane and a high electrode compression ratio of 62.5%, the operating current density of the ICRFB can reach as high as 480 mA cm^{-2} at an energy efficiency of higher than 80%; (ii) the bismuth catalyst loading has insignificant effect on the battery performance in the range of 0.52–10.45 mg cm^{-2}; (iii) the moderately oxidative thermal pretreatment of the electrode improves the energy efficiency compared to the as-received electrode while the electrode prepared with a harsh pretreatment deteriorates the battery performance; and (iv) for the present ICRFBs operating at both 25 and 65 °C, the dominant loss is identified to be ohmic loss rather than kinetics loss.

17/02026 Thermal behavior and failure mechanism of lithium ion cells during overcharge under adiabatic conditions
Ye, J. *et al. Applied Energy*, 2016, 182, 464–474.
Cells in battery packs are easily overcharged when battery management system (BMS) is out of order, causing thermal runaway. However, the traditional calorimetry could not estimate dynamic overcharging heat release. In this study, commercial $LiCoO_2 + Li(Ni_{0.5}Co_{0.2}Mn_{0.3})O_2$/$C + SiO_x$ cells are employed to investigate the dynamic thermal behaviours during overcharge under adiabatic condition by combining a multi-channel battery cycler with an accelerating rate calorimeter. The results indicate that overcharging with galvanostatic–potentiostatic–galvanostatic regime is more dangerous than that with galvanostatic way. Side reactions contribute 80% heat to thermal runaway in cases below 1.0 C charging rate. To prevent the thermal runaway, the effective methods should be taken within 2 min to cool down the batteries as soon as the cells pass inflection point voltage. Hereinto, the inflection and maximum voltages increase linearly with the increasing current rates. By scanning electron microscope and energy dispersive spectrometer, the decomposed products of cathode materials are suspected to be soluble with SiO_x. The overcharge induced decomposition reaction of $Li(Ni_{0.5}Co_{0.2}Mn_{0.3})O_2$ is also proposed. These results can provide support for the safety designs of lithium ion batteries and BMS.

17/02027 Tube-like carbon for Li-ion capacitors derived from the environmentally undesirable plant: *Prosopis juliflora*
Sennu, P. *et al. Carbon*, 2016, 98, 58–66.
This work describes the fabrication of high-energy Li-ion hybrid electrochemical capacitors (Li-HEC) from the environmentally threatening and invasive *Prosopis juliflora*. The carbon derived from this acts as the positive electrode active material in organic medium. High-surface-area carbon was obtained from *P. juliflora* and activated using KOH at various concentrations and temperatures. Of the tested ratios, 1 : 2 (carbon : KOH) treated at 900 °C (KC21-900) yielded a high specific surface area (2410 $m^2 g^{-1}$) and specific capacitance (~161 F g^{-1}). Then, a Li-HEC was fabricated with a homemade insertion-type $Li_4Ti_5O_{12}$ negative electrode, delivering a maximum energy density of ~80 W h kg^{-1}. In addition, the prepared Li-HEC had excellent cycleability (10,000 cycles) and good capacity retention characteristics.

12 REFRACTORIES/ CERAMICS

Properties, production, applications

17/02028 A 3.2% output increase in an existing photovoltaic system using an anti-reflection and anti-soiling silica-based coat
Ota, Y. *et al. Solar Energy*, 2016, 136, 547–552.
The amount of radiation received by the solar cells inside a photovoltaic (PV) module is lower than that arriving at the module surface, owing to reflection and soiling of the module surface. To develop high-efficiency PV systems, these effects must be addressed. In this study, a silica-based layer with anti-reflection and anti-soiling properties was coated onto the surface of a $Cu(In, Ga)Se_2$ PV module and the effects were assessed. The coating method was simple, allowing it to be applied to already installed PV modules. The cleaning and coating treatments were carried out on 25 December 2014, and the arrays were exposed outdoors for 7 months to investigate the effects of the treatment. The output of the array that received the coating was 3.2% greater than that of an uncoated array. It was also found that the coating reduced the reflection of the light entering from a high incident angle.

17/02029 A comparative study on the effect of glazing and cooling for compound parabolic concentrator PV systems – experimental and analytical investigations
Bahaidarah, H. M. *et al. Energy Conversion and Management*, 2016, 129, 227–239.
A key barrier to achieving the economic viability and widespread adoption of photovoltaic (PV) technology for the direct conversion of solar radiation to electricity is the losses related to the high operating temperatures of typical flat-type PV modules. This technical and economic study addresses the cost reduction of PV systems by proposing a methodology for the improvement of solar cell efficiency using low-concentration PV technology and compound parabolic concentrators (CPCs). A theoretical model was developed to evaluate the performance of PV-CPC systems considering their optical, thermal and electrical properties. The model was implemented to investigate glazed and unglazed PV-CPC systems with and without active cooling and it was validated against experimental data. A laboratory-scale bench-top PV string was designed and built with symmetrically truncated CPC modules in these four configurations. The constructed glazed and unglazed PV-CPC systems were used for measurements at the geographic location of Dhahran and showed a very good agreement of 3.8–6.5% between the calculated and experimental results. The effect of glazing was studied and from the electrical point of view, glazing was found to reduce the power output. From the thermal point of view, glazing increased the thermal gain of the PV-CPC system. An unglazed PV-CPC system is recommended for greater electric power output, and glazed system is recommended for higher thermal gain. For economic feasibility, levelized cost of energy (LCE) analysis was performed using annual power output simulations and cost parameters incurred in the installation and operations phase of four systems considered. Annual power output was found to increase by 53.45% for unglazed CPC and 37.1% for glazed CPC systems. The minimum LCE of 0.84 (€/kW h) was found for unglazed CPC with cooling whereas the maximum LCE of 1.67(€/kW h) was obtained for glazed uncooled system due to high cell temperatures.

17/02030 A study on the reduction of $CaCO_3$ fouling in hot-water storage tank by short pulse plasma application (rev 1 yc)
Nam, H. *et al. Applied Thermal Engineering*, 2016, 102, 108–114.
The present study investigated the feasibility of using plasma spark discharge to prevent mineral fouling on the coil heat exchanger in a hot-water storage tank, which is used in a large heat pump system. Experimental fouling test was conducted with spark discharges produced directly in water inside the tank. The overall heat transfer coefficient was determined from both flow rate and four temperatures measured at the inlet and outlet of the coil heat exchanger. The artificial hard water was used to accelerate the fouling process on the heat exchanger surface. The test results showed that the fouling in the coil heat exchanger was effectively suppressed using plasma application. For the case of 1250-ppm solution, the fouling resistance was reduced by 66% with plasma application compared with no-treatment case. The spark discharge plasma application can be a useful method to reduce the mineral fouling on the coil heat exchanger in a hot-water storage tank.

17/02031 Anode properties of silicon-rich amorphous silicon suboxide films in all-solid-state lithium batteries
Miyazaki, R. *et al. Journal of Power Sources*, 2016, 329, 41–49.
This paper reports the effects of introducing oxygen into amorphous silicon films on their anode properties in all-solid-state lithium batteries. Although poor cycling performance is a critical issue in silicon anodes, it has been effectively improved by introducing even a small amount of oxygen, that is, even in Si-rich amorphous silicon suboxide (a-SiO_x) films. Because of the small amount of oxygen in the films, high cycling performance has been achieved without lowering the capacity and power density: an a-Si film delivers discharge capacity of 2500 mAh g^{-1} under high discharge current density of 10 mA cm^{-2}(35 C). These results demonstrate that a-SiO_x is a promising candidate for high-capacity anode materials in solid-state batteries.

17/02032 Application of glass beads as retro-reflective facades for urban heat island mitigation: experimental investigation and simulation analysis
Yuan, J. *et al. Building and Environment*, 2016, 105, 140–152.

Glass beads are the common main component of retro-reflective (RR) material applied to building envelopes for urban heat island (UHI) mitigation. In order to evaluate the influence of glass bead RR materials on the UHI mitigation, two glass bead RR samples with refractive index of 1.9 and 1.5 in white reflective layer, one prism RR sample and one white diffusive sample for comparison were produced for this study. Their RR angular distributions of reflection intensity were investigated by an emitting-receiving optical fibre system developed in the laboratory. Their solar reflectance at different incident angles was measured by thermal balance theory in the outdoor environment. Furthermore, the influence of these developed samples on UHI mitigation potential was evaluated at an example location of Osaka, Japan using a 2-D analytic model. It showed that the glass bead RR sample with refractive index of 1.9 is more effective for mitigating the UHI phenomenon, both increasing the urban albedo and reducing the proportion of solar radiation absorbed by urban canyons.

17/02033 Axial friction response of full-scale pipes in soft clays

Wang, J. and Yang, Z. *Applied Ocean Research*, 2016, 59, 10–23.

The axial friction response of subsea pipelines in soft clays is a very important aspect for designers of subsea pipelines but the response is not well understood so far. There is a pressing need for the comprehension of the response. In this paper, model tests are performed using full-scale pipes coated with polyethylene (PE) to study the effects of the set-up period, the pipe diameter, the buried depth of the pipe, the shear strength of soft clays and the loading rate on the axial friction response of pipelines in soft clays. The variations of the axial friction coefficient are analysed using the effective stress method based on model test results. The results show that the axial friction resistance increases with the increasing pipe diameter but the effect of the pipe diameter on the axial friction coefficient can be neglected. The ultimate axial resistance also increases with the increase of the buried depth of pipelines, the undrained shear strength of soft clays and the loading rate. The axial friction coefficient increases with the increasing loading rate. However, the axial friction coefficient decreases with the increasing buried depth. The method to determine the axial friction coefficient is developed by analysing model test results, which considers the effects of the diameter, the buried depth, the undrained shear strength of soft clays and the loading rate. The study results not only extend the industry data base but also supply a basis to determine the axial friction coefficient of PE-coated pipes in soft clays for ocean engineering geological investigations.

17/02034 Optical model for multilayer glazing systems: experimental validation through the analytical prediction of encapsulation-induced variation of PV modules efficiency

Machado, M. *et al. Solar Energy*, 2016, 135, 77–83.

A simple analytical calculation based on a transfer matrix method for incoherent optics, allowing the prediction of photovoltaic module efficiencies in different encapsulation conditions is presented. This approach is used for the experimental validation of the main features of the optical model for multilayer glazing systems considered, through the relation between the external quantum efficiency of the module and its optical modelling. The theoretical procedure avoids the need to manufacture and characterize by solar simulator or external quantum efficiency measurements all the variety of photovoltaic module configurations, which is of interest at research and manufacturing levels, especially for building-integrated photovoltaics. The absorptivity of encapsulated solar cells is not directly accessible from direct air-bare cell or air-encapsulated cell optical measurements, and therefore analytical or numerical methods are generally needed. The calculations presented in this work provide closed analytical expressions for the layer-by-layer absorption of the different components of a photovoltaic module. From a small set of experimental measurements of a particular encapsulation configuration, and the theoretical expressions for spectral absorptivities, the short-circuit current of a module can be predicted for any other encapsulation scheme. It will be proved that the method accurately matches short-circuit current density of the modules as obtained from experimental measurements. Results will be presented for crystalline silicon and CIGS thin film cell technologies with several glass and encapsulation material combinations.

17/02035 Porosity and insulating properties of silica-fume based foams

Papa, E. *et al. Energy and Buildings*, 2016, 131, 223–232.

The synthesis of silica-fume based foams, with a multi-range macro-porosity, was obtained by alkaline activation. Foams were obtained through an *in situ* foaming process exploiting the gaseous production of hydrogen caused by the oxidation, in alkaline medium, of metal silicon impurities contained in silica fume. Potassium or sodium alkaline solutions were selected and a temperature of 70 °C was sufficient to promote the development of hydrogen bubbles, the increase of the viscosity and the consolidation of the foams. The balance of these reactions allowed to entrap hydrogen bubbles inside the structures creating highly porous foams. The foams were characterized in term of macro- and microstructure, porosity distribution, infrared spectroscopy, thermal and acoustic properties achieved. The foams showed ultra-macroporous structures, with a total porosity of ≈80%. The average values of bulk density ($0.5\,g\,cm^{-3}$), thermal conductivity ($0.16\,W\,m^{-1}\,K^{-1}$), and the acoustic behaviours, highlighted a use of the foams as promising insulating materials.

17/02036 Portable solar spectrum reflectometer for planar and parabolic mirrors in solar thermal energy plants

Salinas, I. *et al. Solar Energy*, 2016, 135, 446–454.

This contribution presents a new field solar spectrum reflectometer for solar-weighted specular reflectance characterization of planar, spherical or parabolic mirrors. This reflectometer is designed to provide fast and reliable field measurements and to be valid for any type of mirror currently installed in concentrated solar power systems, including parabolic trough, Stirling dish and central receiver power plants. The optical design of the solar spectrum reflectometer, which includes six LEDs in the VIS–NIR band, is described, and its tolerance to variations in the geometrical parameters of the mirrors discussed and evaluated. The contribution of diffuse reflection and its impact on the measured reflectance is also calculated for different concentrated solar power systems.

17/02037 Si nanoparticles/graphene composite membrane for high performance silicon anode in lithium ion batteries

Luo, Z. *et al. Carbon*, 2016, 98, 373–380.

Silicon is an exciting anode material with high specific capacity of $4200\,mAh\,g^{-1}$, which is more than ten times the theoretical capacity of the commercialized graphite anode. However, successful applications of Si anode have been impeded by rapid capacity fading caused by large volume expansion (pulverization and subsequent electrical disconnection) during lithiation/delithiation and low ionic/electronic conductivity. Tackling the Si anode problems require a multifaceted design, which can simultaneously address the above-mentioned problems of Si-based anode. Here, the authors present a facile approach to fabricate the freestanding Si/graphene composite membrane for Si anode in a large scale, allowing control over uniformly inserting Si nanoparticles into the pores between graphene sheets from nanoscale to macroscale. They demonstrate its high specific discharge capacities and excellent capacity retention. Over a long-term cycling of 1300 cycles at $400\,mA\,g^{-1}$, a capacity decay as low as 0.06% per cycle and an average Coulombic efficiency of 99.8% was achieved.

17/02038 Silica decorated on porous activated carbon nanofiber composites for high-performance supercapacitors

Kim, S. Y. and Kim, B.-H. *Journal of Power Sources*, 2016, 328, 219–227.

A hybrid of silica decorated on porous activated carbon nanofibres (ACNFs) is fabricated in the form of a web via electrospinning and an activation process as an electrode material for electrochemical capacitors in an organic electrolyte. The introduction of $PhSiH_3$ (PS) into the polyacrylonitrile (PAN) solution induces a porous ACNF structure containing silica nanoparticles (NPs) via the spontaneous sol-gel process of PS by steam in the subsequent physical activation process. These inorganic-organic hybrid composites of porous ACNF containing silica NPs show superior specific capacitance and energy density in electrochemical tests, along with good rate capability and excellent cycle life in an organic electrolyte, which is attributed to the combination of ACNF's high surface area and silica's hydrophilicity. The electrochemical performance decreases with increasing PS concentration, and this trend is consistent with the specific surface area results, which reveal the rapid formation of a double layer.

17/02039 Statistical analysis and engineering fit models for two-diode model parameters of large area silicon solar cells

Khanna, V. *et al. Solar Energy*, 2016, 136, 401–411.

In this paper, an attempt has been made to find the correlation between various parameters of the two-diode equivalent circuit model of silicon solar cells. The statistical analysis has been done to find the engineering fit models between these parameters. The solar cell parameter data of 82 solar cell samples has been estimated using the particle swarm optimization method from the measured illuminated *I–V* characteristics of the cells. This data on estimated parameters has been used to find the Pearson's correlation coefficient between different parameters and the significant outcome of this work is that it revealed a high correlation between the first diode's reverse saturation current and its ideality factor and a medium correlation between the second diode's reverse saturation current and its ideality factor in the two-diode equivalent circuit model of a silicon solar cell. An engineering fit model has been suggested between the reverse saturation current and ideality factor of the first diode, based on the

data of 82 large area (~154.8 cm^2) silicon solar cells with AM1.5 conversion efficiency between 15% and 18.4%. The suggested engineering fit between the two would be a method to reduce the number of parameters needed for silicon solar cell modelling and to make it easier for predicting the module output.

17/02040 Thermal evaluation of a double glazing façade system with integrated parallel slat transparent insulation material (PS-TIM)
Sun, Y. *et al. Building and Environment*, 2016, 105, 69–81.
Concerns over sustainability in the built environment have resulted in continuous efforts to improve the performance of glazed façade systems and hence indoor comfort and building energy conservation. An innovative façade system where parallel transparent plastic slats are sandwiched between glass panes to form a parallel slat transparent insulation material (PS-TIM) is proposed as a strategy to effectively reduce coupled convective and radiative heat transfer between the panes of a double glazed window. This strategy increases the thermal resistance of the façade, while maintaining access to daylight. A numerical investigation of the thermal and optical performance of this façade system is presented. Detailed modelling of the thermal characteristics of a double glazed window containing PS-TIM systems was carried out for different cell aspect ratios (defined by the thickness of window air cavity and slat interval distance), slat thickness and slat properties (conductivities and emissivities) using a validated computational fluid dynamics (CFD) model. The CFD predictions show that: (1) an aspect ratio of 0.35 can provide full suppression of convection; (2) the PS-TIM structure can achieve a 35–46% reduction in thermal conductance compared with the same double glazing in the absence of PS-TIM; (3) material conductivity, thickness and emissivity have a more apparent influence on small cell structures than large cell structures. In addition, a simple analysis of U-value and light transmittance at various solar incidence angles was undertaken. The results provide a better understanding of the benefits of PS-TIM in terms of energy saving and offer suggestions for the improved design of glazing façade systems.

17/02041 Three-dimensional minority-carrier collection channels at shunt locations in silicon solar cells
Guthrey, H. *et al. Solar Energy*, 2016, 135, 163–168.
This study demonstrates the value of using a multiscale multi-technique characterization approach to study the performance-limiting defects in multi-crystalline silicon (mc-Si) photovoltaic devices. The combination of dark lock-in thermography (DLIT) imaging, electron beam induced current imaging, and both transmission and scanning transmission electron microscopy (TEM/STEM) on the same location revealed the nanoscale origin of the optoelectronic properties of shunts visible at the device scale. The site-specific correlative approach identified the shunt behaviour to be a result of three-dimensional inversion channels around structural defects decorated with oxide precipitates. These inversion channels facilitate enhanced minority-carrier transport that results in the increased heating observed through DLIT imaging. The definitive connection between the nanoscale structure and chemistry of the type of shunt investigated here allows photovoltaic device manufacturers to immediately address the oxygen content of their mc-Si absorber material when such features are present, instead of engaging in costly characterization.

17/02042 Time evolution of graphene growth on SiC as a function of annealing temperature
Zarotti, F. *et al. Carbon*, 2016, 98, 307–312.
The authors used X-ray photoelectron spectroscopy to follow the time evolution of graphene layers obtained by annealing 3C SiC(111)/Si(111) crystals at different temperatures. The intensity of the carbon signal provides a quantification of the graphene thickness as a function of the annealing time, which follows a power law with exponent 0.5. It is shown that a kinetic model, based on a bottom-up growth mechanism, provides a full explanation to the evolution of the graphene thickness as a function of time, allowing to calculate the effective activation energy of the process and the energy barriers, in excellent agreement with previous theoretical results. This study provides a complete and exhaustive picture of Si diffusion into the SiC matrix, establishing the conditions for a perfect control of the graphene growth by Si sublimation.

13 ALTERNATIVE ENERGY SUPPLIES

Biofuels and bioconversion energy

17/02043 A bio-based 'green' process for catalytic adipic acid production from lignocellulosic biomass using cellulose and hemicellulose derived γ-valerolactone
Han, J. *Energy Conversion and Management*, 2016, 129, 75–80.
A bio-based 'green' process is presented for the catalytic conversion of corn stover to adipic acid (ADA) based on experimental studies. ADA is used for biobased nylon 6.6 manufacturing from lignocellulosics as carbon and energy source. In this process, the cellulose and hemicellulose fractions are catalytically converted to γ-valerolactone (GVL), using cellulose and hemicellulose-derived GVL as a solvent, and subsequently upgrading to ADA. Experimental studies showed maximal carbon yields (biomass-to-GVL: 41% and GVL-to-ADA: 46%) at low concentrations (<16 wt% solids) using large volumes of GVL solvents while requiring efficient interstage separations and product recovery. This work presents an integrated process, including catalytic conversion and separation subsystems for GVL and ADA production and recovery, and designs a heat exchanger network to satisfy the total energy requirements of the integrated process via combustion of biomass residues (lignin and humins). Finally, an economic analysis shows that 2000 tonnes per day of corn stover feedstock processing results in a minimum selling price of $633/tonne if using the best possible parameters.

17/02044 A comparison of the energy use of *in situ* product recovery techniques for the acetone butanol ethanol fermentation
Outram, V. *et al. Bioresource Technology*, 2016, 220, 590–600.
The productivity of the acetone butanol ethanol (ABE) fermentation can be significantly increased by application of various *in situ* product recovery (ISPR) techniques. There are numerous technically viable processes, but it is not clear which is the most economically viable in practice. There is little available information about the energy requirements and economics of ISPR for the ABE fermentation. This work compares various ISPR techniques based on UniSim process simulations of the ABE fermentation. The simulations provide information on the process energy and separation efficiency, which is fed into an economic assessment. Perstraction was the only technique to reduce the energy demand below that of a batch process, by approximately 5%. Perstraction also had the highest profit increase over a batch process, by 175%. However, perstraction is an immature technology, so would need significant development before being integrated to an industrial process.

17/02045 A fuzzy information axiom based method to determine the optimal location for a biomass power plant: a case study in Aegean region of Turkey
Cebi, S. *et al. Energy*, 2016, 116, 894–907.
Biomass energy is one of the fundamental renewable energy sources. It decreases fossil fuel combustion and consequently net greenhouse gas emissions since no new carbons are not released to the atmosphere. Generally, agricultural, forest, animal and urban wastes are considered as potential sources for biomass energy. Among these sources, agricultural wastes are the most suitable type to generate biomass energy in Turkey. The Aegean region has a great potential with respect to its lands and its diversity of agricultural products. In this paper, the most appropriate location for a biomass power plant has been investigated among the eight alternative locations in the Aegean region by examining both quantitative and qualitative criteria. It is the first time, an integrated model including fuzzy sets, analytic hierarchy process, opinion aggregation method, and information axiom method has been proposed to obtain a solution for such a problem. According to the results, *Aydin* is determined as the most appropriate location for a biomass power plant at Aegean Region. Furthermore, a sensitivity analysis has been performed to present the reliability of the obtained results.

17/02046 A spreadsheet calculator for estimating biogas production and economic measures for UK-based farm-fed anaerobic digesters
Wu, A. *et al. Bioresource Technology*, 2016, 220, 479–489.
This paper presents a spreadsheet calculator to estimate biogas production and the operational revenue and costs for UK-based farm-fed anaerobic digesters. There exist sophisticated biogas pro-

duction models in published literature, but the application of these in farm-fed anaerobic digesters is often impractical. This is due to the limited measuring devices, financial constraints, and the operators being non-experts in anaerobic digestion. The proposed biogas production model is designed to use the measured process variables typically available at farm-fed digesters, accounting for the effects of retention time, temperature and imperfect mixing. The estimation of the operational revenue and costs allow the owners to assess the most profitable approach to run the process. This would support the sustained use of the technology. The calculator is first compared with literature reported data, and then applied to the digester unit on a British farm to demonstrate its use in a practical setting.

17/02047 An integrated system for fractionation and hydrolysis of sugarcane bagasse using heterogeneous catalysts in aqueous biphasic system

Sakdaronnarong, C. *et al. Chemical Engineering Journal*, 2016, 285, 144–156.

Sugarcane bagasse fractionation and hydrolysis using heterogeneous catalysts in aqueous biphasic system was investigated. Carbon-based, polymer-based and metal-based catalysts were synthesized and tested for hydrolysis of sugarcane bagasse in a combination of solvent-based and polymer-based aqueous biphasic system at different polarities for sugar production. The results showed that acid density, functional groups and physical properties of catalysts influenced the catalytic activity on cellulose hydrolysis. From solvent screening study, nitrobenzene was the most promising solvent enhancing relatively high total reducing sugar (TRS) yield of 97.4% when hydrolysis took place at 140 °C for 4 h in the presence of carbon-based catalyst type 1(C-SO_3H). Nevertheless in terms of recyclability, magnetic metal-based catalyst ($SO_4^{2-}/TiO_2/Fe_3O_4$) that yielded considerably high amount of glucose at elevated temperature and shorter time (180 °C for 1 h) was suitable catalyst as it was easily separated from the solution. Kinetic study of cellulose hydrolysis reaction was performed, in which rate constant and activation energy of reaction catalysed by active catalysts were compared. The results suggested an effective integrated system for cellulose fractionation and hydrolysis in which lignin-rich fraction was in solvent and polymer phases while cellulose fibres were remained in the aqueous phase and further hydrolysed by heterogeneous catalyst.

17/02048 Biomass derivative/graphene aerogels for binder-free supercapacitors

Song, W.-L. *et al. Energy Storage Materials*, 2016, 3, 113–122.

Advanced self-supported electrode materials of various morphologies have recently presented bendable, stretchable and processable features with exceptional application potential in flexible and wearable energy storage devices. Although biomasses and related wastes as abundant natural sources are the ideal low-cost raw materials, their derivatives generally suffer from insufficiently electrically conductive or inadequately mechanically robust, which is generally required to be further processed into electrodes with binders and conductive agents. To break through such barrier, in this contribution, a universal approach is reported to manipulate the three-dimensional (3D) biomass-derived carbon networks into binder-free supercapacitors using *in situ* graphene aerogel. Such interfacial management has shown remarkable improvements in the chemical composition, surface area and pore size distribution, enabling the self-supported biomass-derived carbon network/graphene aerogel of hierarchical 3D interconnected structures to deliver considerable enhancement in the charge transfer and capacitive storage (up to 320 and 200 $F\,g^{-1}$ at 0.1 and 10 $A\,g^{-1}$, respectively). The results of the binder-free flexible all-solid state devices and electrical power based on three devices in the series circuit promise an exceptionally universal stage for engineering advanced energy storage devices with rich natural sources as well as recycling biomasses and wastes for extended applications.

17/02049 Characteristics and deoxy-liquefaction of cellulose extracted from cotton stalk

Li, J. *et al. Fuel*, 2016, 166, 196–202.

Cellulose was extracted from cotton stalk and characterized by using scanning electron microscope, X-ray diffraction, nuclear magnetic resonance, and Fourier transform infrared (FTIR) spectroscopy. The results showed that the extracted cellulose had representative cellulose structure. Furthermore, the extracted cellulose was converted into liquid oil by direct deoxy-liquefaction. The elemental analysis, FTIR spectroscopy and gas chromatography–mass spectrometry analyses of the liquid oil indicated that the extracted cellulose oil was mainly composed of aromatic hydrocarbons, phenols and alkanes. This oil featured high quality including the low oxygen content of 6.46% and the higher heating value of 42.66 MJ/kg. This suggested that deoxy-liquefaction technique may be an effective way to convert cellulose into high-quality liquid fuel and value-added chemicals.

17/02050 Characterization and parametric study of mesoporous calcium titanate catalyst for transesterification of waste cooking oil into biodiesel

Yahya, N. Y. *et al. Energy Conversion and Management*, 2016, 129, 275–283.

Mesoporous calcium titanate (MCT) catalyst was synthesized via a sol-gel-hydrothermal method and investigated as a catalyst for biodiesel production from waste cooking oil (WCO). Calcium was supported on titanate in order to increase their surface area, stability and consequently, improve its performance in the transesterification of WCO to biodiesel. Synthesized catalyst was characterized with powder X-ray diffraction, field emission scanning electron microscopy, N_2 physisorption, Fourier transform-infrared spectroscopy, thermogravimetric analysis and carbon dioxide temperature-programmed desorption. The catalyst possessed high surface area, basicity and stability than calcium oxide catalyst. The highest biodiesel yield achieved was 80.0% in 3 : 1 of methanol to WCO molar ratio, 0.2 wt% of MCT catalyst for 1 h at 65 °C. Reusability study suggested that this catalyst can be recycled for five successive runs.

17/02051 Co-torrefaction of sewage sludge and leucaena by using microwave heating

Huang, Y.-F. *et al. Energy*, 2016, 116, 1–7.

Microwave co-torrefaction of sewage sludge and leucaena can be a workable technique, because it not only produces biofuels but also solves the problems in waste treatment. When the sewage sludge blending ratio was 25–50 wt% and the microwave power level was 100 W, a synergistic effect was found to influence the mass and energy yields as well as product properties. The relatively small amount of sewage sludge could play a role as a catalyst, since the synergistic effect was hard to be identified at higher sewage sludge blending ratios. Besides, it was difficult to find out the synergistic effect at higher microwave power levels. This could be attributable to the effect of microwave heating which increases with its power level. The elemental compositions of biochar were close to those of anthracite and bituminous coal. The energy return on investment (EROI) of microwave co-torrefaction of the 25/75 (w/w) sewage sludge/leucaena blend at a microwave power level of 100 W in a processing time of 30 min can be approximately 10.1 or 4.7, when the gaseous and liquid products are utilized or not. Therefore, the technique should be energetically and economically feasible.

17/02052 Comparative analysis of top-lit bubble column and gas-lift bioreactors for microalgae-sourced biodiesel production

Hosseini, N. S. *et al. Energy Conversion and Management*, 2016, 130, 230–239.

The development of top-lit 1-metre deep bioreactors operated as either a gas-lift or bubble column system using air and carbon dioxide enriched air was studied. The goal was high productivity cultivation of algae with elevated lipid levels suitable for conversion into biodiesel. A theoretical energy requirement analysis and a hydrodynamic model were developed to predict liquid circulation velocities in the gas-lift bioreactor, which agreed well with experimental measurements. The influence of operational parameters such as design of bioreactor, gas flow rates and carbon dioxide concentration on the growth and lipid volumetric production of *Scenedesmus dimorphus* was evaluated using factorial design. While biomass productivity was 12% higher in the bubble column bioreactor (68.2 $g_{dw}\,m^{-2}\,day^{-1}$), maximum lipid volumetric production (0.19 $g_{Lipid}\,L^{-1}$) was found in a gas-lift bioreactor sparged with 6% carbon dioxide due to hydrodynamic and light stresses.

17/02053 Comparative biogas generation from fruit peels of fluted pumpkin (*Telfairia occidentalis*) and its optimization

Dahunsi, S. O. *et al. Bioresource Technology*, 2016, 221, 517–525.

This study evaluated the potentials of fluted pumpkin fruit peels for biogas generation using three different pre-treatment methods (A, B, C) and the optimization of its process parameters. The physico-chemical characteristics of the substrates revealed it to be rich in nutrients and mineral elements needed by microorganisms. Gas chromatography analysis revealed the gas composition to be within the range of $58.5 \pm 2.5\%$ methane and $27 \pm 3\%$ carbon dioxide for all the three digestions. The study revealed that combination of three pre-treatment methods enhanced enormous biogas yield from the digested substrates as against the use of two methods and no pre-treatment experiment. Optimization of the generated biogas data revealed that response surface methodology predicted higher gas yield than artificial neural networks, the latter gives higher accuracy and efficiency than the former. It is advocated that fluted pumpkin fruit peels be used for energy generation especially in the locations of its abundance.

17/02054 Comparing the influence of acetate and chloride anions on the structure of ionic liquid pretreated lignocellulosic biomass

Kim, H. *et al. Biomass and Bioenergy*, 2016, 93, 243–253.

The effect of the anion type, in an ionic liquid, on the transition of the crystalline structure when lignocellulose was pretreated in 1-ethyl-3-methylimidazolium acetate (EmimOAC) or 1-ethyl-3-methylimidazolium chloride (EmimCl) was studied. The influence of the pretreatment on the composition, the molecular structure, and the crystalline structure was observed using Fourier-transform infrared compositional analysis, thermogravimetric analysis, rheological behaviour and X-ray diffraction. Compared to EmimCl, EmimOAC pretreatment substantially decreased the lignin and hemicellulose contents. The pretreatment also significantly changed the entanglement or crosslinking state of polymer chains in the lignocellulose solution. The changes in lignin content and the transformation from cellulose I to II were dependent on the anion type of the ionic liquid. The pretreated samples were recrystallized to cellulose II only in EmimOAC, whereas the samples pretreated with EmimCl had both cellulose I and II structures present at the same time.

17/02055 Droplet combustion characteristics of algae-derived renewable diesel, conventional #2 diesel, and their mixtures

Xu, Y. *et al. Fuel*, 2016, 167, 295–305.

Fuels derived from bio-feedstocks have received significant attention for their potential to reduce the consumption of petroleum-based liquid fuels, either through blending or direct use. Biofuels produced from heterotrophic microalgae are particularly attractive because of fast conversion of sustainable plant sugars into renewable oils of controllable quality and composition, but without the need for sunlight or carbon from the atmosphere for growth. This paper describes the results of a fundamental study of the combustion characteristics of hydroprocessed renewable diesel fuel (HRD) produced from this strain of algae, and the results are compared to #2 diesel fuel (DF2) and an equi-volume mixture of HRD and #2 diesel (R50) as representative of blending. A canonical combustion configuration is used for a liquid fuel consisting of an isolated droplet burning with spherical symmetry and with fuel transport being entirely the result of evaporation at the droplet surface. This fundamental liquid fuel burning configuration is conducive to articulating the evaporation and sooting dynamics involved. The results show that combustion rates and relative positions of the flame and soot aggregates to the droplet surface of HRD droplets are quite close to R50 and DF2 in spite of their significant chemical and sooting differences. These trends are explained based on similarities in the thermal properties of the fuels. Sooting propensity of #2 diesel is greater than that of HRD, with the mixture falling qualitatively in-between. The results suggest that HRD derived from heterotrophic microalgae can potentially be considered a drop-in replacement for DF2 or serve as an additive to DF2.

17/02056 Economic-energy-environment analysis of prospective sugarcane bioethanol production in Brazil

de Carvalho, A. L. *et al. Applied Energy*, 2016, 181, 514–526.

Bioethanol from sugarcane can be produced using first-generation (1G) or second-generation (2G) technologies. 2G technologies can increase the capacity of production per sugarcane mass input and are expected to have a key role in future reductions of environmental impacts of sugarcane bioethanol. A hybrid input–output (IO) framework is developed for Brazil coupling the system of national accounts and the national energy balance, which is extended to assess greenhouse gas (GHG) emissions. Life-cycle based estimates for two sugarcane cultivation systems, two 1G and eight 2G bioethanol production scenarios, are coupled in the IO framework. A multi-objective linear programming (MOLP) model is formulated based on this framework for energy-economic-environmental analysis of the Brazilian economic system and domestic bioethanol supply in prospective scenarios. Twenty-four solutions are computed: four 'extreme' solutions resulting from the individual optimization of each objective function (GDP, employment level, total energy consumption and total GHG emissions – 1G scenario), 10 compromise solutions minimizing the distance of the feasible region to the ideal solution (1G, 1G-optimized and prospective 1G + 2G scenarios), and 10 solutions maximizing the total bioethanol production (1G, 1G-optimized and prospective 1G + 2G scenarios). Higher diesel oil and lubricants consumption in the mechanical harvesting process has counterbalanced the positive effects of more efficient trucks leading to higher energy consumption and GHG emissions. Lower overall employment level in the 1G + 2G scenarios is achieved such that policies linked to reabsorption of sugarcane cutters in alternative activities are positive. Indirect effects from maximizing the bioethanol production increase the total energy consumption and the GHG emissions thus requiring efficiency measures and fossil energy substitution by cleaner sources. The integrated- or country-based analysis of the whole economic system has complemented the process design and process-based analysis, contributing to identify direct and indirect effects that can offset the benefits. Direct and indirect effects on the whole economic system have to be considered in policies and technological choices for prospective bioethanol production, since positive direct effects of 1G + 2G plants can be counterbalanced by indirect impacts on other sectors, mainly from chemicals in the process.

17/02057 Effect of freeboard deflectors in the fixed bed combustion of biomass

Rashidian, B. *et al. Applied Thermal Engineering*, 2016, 103, 543–552.

Deflectors have been used in the freeboard section of industrial combustors to reduce radiant heat loss through flue gases and for particle emissions abatement. Freeboard deflectors can also reduce the draft force of flue gases and affect flow dynamics. There have been no systematic studies to investigate the effects of deflectors on the temperature profiles and emissions in laboratory scale fixed bed biomass combustors. This research includes experiments conducted over lean conditions (λ_{total}) on fixed bed combustor, with a freeboard deflector located at different axial locations. The aim is to characterize the effects on temperature distribution (near-wall and near-centreline) and gaseous emissions (NO, CO, CO_2) over a range of primary and secondary air flow rates. Experimental results indicate that deflectors affect upstream near-wall temperatures, but their impact depends on relative (axial) position (H). The presence of a freeboard deflector however decreases near-wall temperatures in the downstream which may be due to aerodynamic effects. Deflectors do not appear to affect the centreline temperature profiles downstream of the secondary air. Furthermore, results reveal that deflectors do not have significant effects on the fuel consumption rate when expressed via the burning rate ($kg\,m^{-2}\,s^{-1}$). Results also showed that NO, CO and CO_2 emissions are also affected by the presence of a deflector in the mid-range of combustion stoichiometry ($\lambda_{primary} = 0.439–0.509$). However, deflector effects were found to be most prominent for NO and CO emissions by reducing and rising their levels, respectively.

17/02058 Effect of storage methods on willow chips quality

Krzyżaniak, M. *et al. Biomass and Bioenergy*, 2016, 92, 61–69.

Lignocellulose biomass is a key source of bioenergy in the EU and in Poland. Therefore, this study analysed the effect of the method of storing chips obtained from short rotation willow on their thermo-physical and chemical properties and on the biomass loss, depending on the method of storage and the type of cover, in the climatic conditions of central–eastern Europe. The experiment involved examination of five methods of storage of willow chips: with no cover (control), under permeable covers Toptex 200 and Toptex 300, under vapour-permeable foil and in a wooden shed. The chips were stored from March 2011 to March 2012. Use of cover made of permeable materials was found to improve the biomass quality: its moisture content decreased more than twice and its heating value increased more than twice. The energy content of the stored piles was also found to increase by 10% after a year of storage. The energy content was also found to increase in a roofed pile and to decrease in biomass covered with foil (−9%) and uncovered (−50%). Biomass loss for chips stored under permeable covers ranged from 3.8% to 5.1%. Similar findings were recorded for chips stored in a shed, while the effects were worse for the piles stored under vapour-permeable foil. The worst biomass parameters were recorded for an uncovered pile. Storage of willow chips in an open space under cover could be a cheaper alternative, which could improve the quality of willow chips compared to roofed warehouses.

17/02059 Efficient enzyme-catalysed transesterification of microalgal biomass from *Chlamydomonas* sp.

Choong, W. P. *et al. Energy*, 2016, 116, 1370–1373.

Facing the global issues of dwindling oil reserves and global warming, the search for alternative green energy source has become a priority. Microalgal biofuels has been regarded as a potential sustainable energy source, due to the high oil yield per area of land, ease of culturing microalgae, zero-net carbon emission and reduced competition for arable land. In this paper, five different lipid extraction methods were studied using dry biomass of the microalga *Chlamydomonas* sp. Folch *et al.*'s method gave the highest oil yield of 26.27 wt%. The extracted microalgal oil underwent transesterification process using immobilized lipases. The highest conversion achieved was 72.09% in the following optimized conditions: 0.100 g of immobilized enzymes and solvent to methanol volume ratio of 1 : 1 with tert-butanol as the organic solvent.

17/02060 Emission behaviour of vegetable oil fuel compatible tractors fuelled with different pure vegetable oils

Emberger, P. *et al. Fuel*, 2016, 167, 257–270.

The emission behaviour of pure vegetable oils to be used as a fuel was researched using two vegetable oil fuel compatible tractors. The tractor engines were equipped with a common-rail and pump-line injection system. For the research eight different vegetable oils, one vegetable oil mixture and diesel fuel were used. Vegetable oils are basically

triacylglycerides and can be characterized by the two structure indices average number of carbon atoms (AC) and average number of double bonds (ADB). The results show that both tractors can be operated with vegetable oils and diesel fuel at about the same level of efficiency. Specific test cycle emissions of nitrogen oxides (NO_x) tend to be higher while specific carbon monoxide (CO), hydrocarbon (HC) and particle mass (PM) emissions tend to be lower with the vegetable oils compared to diesel fuel. The emission behaviour of the two tractors was influenced by the type of vegetable oil used. The differences were dependent on the operation mode. At average and high load operation points the emissions of CO, HC and PM were at the same level, whereas the NO_X emissions were rising with increasing ADB of the vegetable oils. At low load and idle operation the emissions of CO, HC and PM were rising with increasing unsaturation respectively increasing ADB of the vegetable oils. The observed increase of NO_X at average and high load could not be recognized anymore at low load and idle and is even reversed for one tractor. This indicates deteriorated combustion with increasing unsaturation of the vegetable oils at idle and low load.

17/02061 Enhanced lipid production in thermo-tolerant mutants of *Chlorella pyrenoidosa* NCIM 2738

Sachdeva, N. *et al. Bioresource Technology*, 2016, 221, 576–587.

The present study aimed to develop thermo-tolerant mutants of *Chlorella pyrenoidosa* NCIM 2738 for high lipids production. For this, ethyl methane sulfonate was used, which generated two effective thermo-tolerant mutants, M18 and M24 of *C. pyrenoidosa* NCIM 2738, capable of surviving at temperature up to 47 °C and showing improved lipid and biomass yields. They showed 59.62% and 50.75% increase, respectively, in lipid content compared to wild type at 30 °C, which could not grow at temperature above 35 °C. The novelty of this study lay in incorporation of PAM fluorometry with mutagenesis to generate thermo-tolerant mutants of *C. pyrenoidosa* and investigating the reasons for increased yields of mutants at cellular and photosynthetic levels with the aim to use them for commercial biodiesel production.

17/02062 Enhancement of biobutanol production by electromicrobial glucose conversion in a dual chamber fermentation cell using *C. pasteurianum*

Mostafazadeh, A. K. *et al. Energy Conversion and Management*, 2016, 130, 165–175.

A set of experiments have been performed to investigate the production of biobutanol as a novel applicable biofuel in a bioelectrolysis cell (BEC). The objective of this work was to understand the mechanism and production rate of the biobutanol by bioelectrosynthesis (BES) using glucose as a substrate. Four main factors, such as electrode materials, substrate concentration, operating temperature, and poised applied voltage were investigated in batch mode to achieve optimum condition for producing maximum butanol by *Clostridium pasteurianum* in BEC. Standard modified P2 medium (MP2) and standard minimal medium (SMM) were used as fermentation media in batch operation mode. Numerical optimization using central composite design (CCD) method has been used to maximize the butanol production within the experimental range. The maximum butanol production 13.31 g/L was obtained by applying 1.32 V indicating the suitability of this procedure. The results showed that by applying optimum conditions in SMM, the butanol could be enhanced remarkably by electroactive microorganisms in cathode chamber.

17/02063 Enhancement of high-solids enzymatic hydrolysis of corncob residues by bisulfite pretreatment for biorefinery

Xing, Y. *et al. Bioresource Technology*, 2016, 221, 461–468.

Co-production of glucose, furfural and other green materials based on a lignocellulosic biorefinery is a promising way to realize the commercial application of corncob residues. An effective process was developed for glucose production using low temperature bisulfite pretreatment and high-solids enzymatic hydrolysis. Corncob residues from furfural production (FRs) were pretreated with 0.1 g $NaHSO_3$/g dry substrate at 100 °C for 3 h. Lignin was sulfonated and sulfonic groups were produced during pretreatment, which resulted in decreasing the zeta potential of the samples. Compared with raw material, bisulfite pretreatment of FRs increased the glucose yield from 18.6 to 99.45% after 72 h hydrolysis at a solids loading of 12.5%. The hydrolysis residues showed a relatively high thermal stability and concentrated high derivatives. Direct pretreatment followed by enzymatic hydrolysis is an environmentally-friendly and economically-feasible method for the production of glucose and high-purity lignin, which could be further converted into high-value products.

17/02064 Enhancing anaerobic digestion of complex organic waste with carbon-based conductive materials

Dang, Y. *et al. Bioresource Technology*, 2016, 220, 516–522.

The aim of this work was to study the methanogenic metabolism of dog food, a food waste surrogate, in laboratory-scale reactors with different carbon-based conductive materials. Carbon cloth, carbon felt and granular activated carbon all permitted higher organic loading rates and promoted faster recovery of soured reactors than the control reactors. Microbial community analysis revealed that specific and substantial enrichments of *Sporanaerobacter* and *Methanosarcina* were present on the carbon cloth surface. These results, and the known ability of *Sporanaerobacter* species to transfer electrons to elemental sulfur, suggest that *Sporanaerobacter* species can participate in direct interspecies electron transfer with *Methanosarcina* species when carbon cloth is available as an electron transfer mediator.

17/02065 Epoxidation of soybean oil at maximum heat removal and single addition of all reactants

de Quadros Jr, J. V. and Giudici, R. *Chemical Engineering and Processing: Process Intensification*, 2016, 100, 87–93.

The epoxidized soybean oil is obtained through the reaction of a lower peracid with the unsaturations of the vegetable oil molecules. The reaction is highly exothermic and temperature control is fundamental to avoid runaway. In industrial practice, a semibatch process is employed, in which performic acid is generated *in situ* by the addition of hydrogen peroxide to oil and formic acid vigorously mixed. Hydrogen peroxide is added gradually as the key procedure to maintain proper temperature control; as a result, the process time is usually long. In the present work the intensification of this process is investigated under conditions of a highly effective heat removal system and all reactants are added at once, thus making the process simpler and faster but still safe. A simple mathematical model was tested to represent the experimental data.

17/02066 Estimation of greenhouse gas (GHG) emission and energy use efficiency (EUE) analysis in rainfed canola production (case study: Golestan province, Iran)

Kazemi, H. *et al. Energy*, 2016, 116, 694–700.

Increasing the use of energy inputs in agricultural section has been led to numerous environmental concerns such as greenhouse gas (GHG) emissions, high consumption of non-renewable resources, loss of biodiversity and environment pollutions. The study was aimed to analyse the energy-use efficiency (EUE) and estimation of GHG emissions from rainfed-based canola production systems (RCPSs) in Iran. In this study, data were collected from 35 farms in Golestan province (north-east Iran) by a face-to-face questionnaire performed and statistical yearbooks of 2014. The amount of GHG emissions (per hectare) from inputs used in RCPSs was calculated using CO_2 emissions coefficient of agricultural inputs. Results showed that the EUE and net energy were as 3.44 and 35,537.81 MJ ha^{-1}, respectively. The value of these indices for the study area indicated that surveyed fields are approximately efficient in the use of energy for canola production. The highest share of energy consumption belonged to nitrogen fertilizer (42.09%) followed by diesel fuel (39.81%). In production of rainfed canola, GHG emission was estimated as 1009.91 kg CO_2 equivalent per hectare. Based on the results, nitrogen fertilizer (44.15%), diesel fuel (30.16%) and machinery (14.49%) for field operations had the highest share of GHG emission. The total consumed energy by inputs could be classified as direct energy (40.09%), and indirect energy (59.91%) or renewable energy (2.02%) and non-renewable energy (97.98%). These results demonstrate that the share of renewable energies in canola production is very low in the studied region and agriculture in Iran is very much dependent on non-renewable energies. In this study, the energy use status in RCPSs has analysed and the main involved causes have been interpreted.

17/02067 GIS-based biomass assessment and supply logistics system for a sustainable biorefinery: a case study with cotton stalks in the southeastern US

Sahoo, K. *et al. Applied Energy*, 2016, 182, 260–273.

Envisioning a sustainable biorefinery requires reliable information on the sustainable availability of biomass, optimal plant location and delivered cost. Here, the authors have developed an integrated geographic information system (GIS)-based sustainable biomass assessment, site optimization and supply logistics cost model to assess the spatial and temporal availability of crop residues, to identify optimal plant sites and to calculate the delivered cost. The grid-level (30 m × 30 m) assessment model was developed for crop residues using three primary sustainability indicators: (1) soil erosion (SE), (2) soil conditioning index (SCI) and (3) crop residue yield $\geq$ 2.5 dry Mg/ha. The artificial neural networks (ANNs) prediction models for each indicator were developed and implemented in the GIS platform to assess sustainably available crop residues. A multi-criteria geospatial analysis was used to identify suitable plant sites. GIS-based location-allocation model was used to site biorefineries/plants at optimal locations and generate feedstock supply curves. The developed model was demonstrated with the sustainable assessment of cotton stalk (CS) to produce fuel pellets in the study region (Georgia, USA). The model

has estimated that about 1.6 million dry Mg of CS is available annually to support seven pellet plants with an average annual plant capacity of 200,000 dry Mg. The average delivered cost of CS ranged between 68 and $75/dry Mg delivered as large rectangular bales with the transport radii ranged from 31 to 60 km. The spatial and temporal variations in the topology and crop yield directly influenced the sustainable availability of CS, the optimal plant location and its capacity and the delivered cost. However, the changes in the optimal plant location and delivered cost were minimal for large capacity plants (>400,000 dry Mg). The developed model can be used to assess multiple crop residues, to manage and control feedstock supply risks and delivered cost variations for a sustainable biorefinery.

17/02068 High-yielding, one-pot, and green production of biodiesel from waste grease using wet cells of a recombinant *Escherichia coli* strain as catalyst

Tian, K. and Li, Z. *Biochemical Engineering Journal*, 2016, 115, 30–37.
Green and efficient production of biodiesel from cheap and non-edible resources is highly desirable. Here the authors develop a practical method for the high-yielding one-pot conversion of low-cost waste grease to biodiesel (FAME) by using wet cells of *Escherichia coli* expressing intracellular *Thermomyces lanuginosus* lipase (TLL) as catalyst. *E. coli* (TLL) was genetically engineered and grew easily to a high cell density with the functional expression of TLL. The easily available and easy to handle wet cells were directly used as catalyst for the biotransformation of waste grease to FAME, with water content of 20–30 wt% (based on grease) and stepwise addition of methanol (4 : 1 molar ratio to grease) as the optimum conditions. Biotransformation of waste grease from Singapore (21 wt% FFA) and Malaysia (9.8 wt% FFA) with 31 wt% wet cells (26 wt% water) gave 99% and 97% FAME yield, respectively. During the biotransformation, the esterification of FFA was faster than the transesterification of triglycerides and the hydrolysis of triglycerides, and nearly no hydrolysis of FAME was observed. Preparative biotransformation was demonstrated to give FAME in >90% yield with a simple isolation procedure. The wet cells were recyclable and retained 55% productivity in the 5th cycle.

17/02069 *In-situ* pyrogenic production of biodiesel from swine fat

Lee, J. *et al. Bioresource Technology*, 2016, 220, 442–447.
In situ production of fatty acid methyl esters (FAME) from swine fat via thermally induced pseudo-catalytic transesterification on silica was investigated in this study. Instead of methanol, dimethyl carbonate (DMC) was used as acyl acceptor to achieve environmental benefits and economic viability. Thermogravimetric analysis of swine fat reveals that swine fat contains 19.57 wt% of water and impurities. Moreover, the fatty acid profiles obtained under various conditions (extracted swine oil + methanol + NaOH, extracted swine oil + DMC + pseudo-catalytic, and swine fat + DMC + pseudo-catalytic) were compared. These profiles were identical, showing that the introduced *in situ* transesterification is technically feasible. This also suggests that *in situ* pseudo-catalytic transesterification has a high tolerance against impurities. This study also shows that FAME yield via *in situ* pseudo-catalytic transesterification of swine fat reached up to 97.2% at 380 °C. Therefore, *in situ* pseudo-catalytic transesterification can be applicable to biodiesel production of other oil-bearing biomass feedstocks.

17/02070 Influence of mill type on densified biomass comminution

Williams, O. *et al. Applied Energy*, 2016, 182, 219–231.
The impact of different mill fracture mechanisms were examined for a wide range of densified biomass pellets to provide a comprehensive analysis of biomass milling behaviour for pulverized fuel combustion. The milling behaviour of seven woody, herbaceous, fruit, and thermally treated densified biomasses were investigated for four distinct types of comminution fracture mechanism using traditional milling indices and novel application of 3D imaging techniques. For the coal mill trials, a reference coal was used to provide a milling performance comparator. For the pre-milled samples, woody and herbaceous pellets have the least spherical particles ($\varphi = 0.324$–0.404), followed by thermally treated pellets ($\varphi = 0.428$), La Loma coal ($\varphi = 0.503$), with olive cake having the most spherical particles ($\varphi = 0.562$). This trend was noted for all the shape factors. Conventional comminution did not significantly impact biomass particle shape, even after a significant change in particle size. Therefore biomass pellet process history plays a key role in determining the comminuted particle shape. La Loma coal had significantly enhanced milling performance in comparison to the biomasses in the coal mills. Significant improvements in grindability and shape factors were observed for the thermally treated pellets. Mill choking was experienced for several of the woody and herbaceous samples, which resulted in a significant energy penalty. The mechanisms of mill choking were found to be intrinsically linked to the critical particle size of comminution through compression, particle shape factors, and the Stokes conditions set for the classifier and burners in pulverized fuel combustion systems. The study showed that for optimal milling performance, biomass pellets should be composed of particles which meet the Stokes requirements of the mill classifier. This would minimize the potential for mill choking and milling energy penalties, and ensure maximum mill throughput.

17/02071 Insight into the solvent, temperature and time effects on the hydrogenolysis of hydrolyzed lignin

Shu, R. *et al. Bioresource Technology*, 2016, 221, 568–575.
The aim of this study is to explore the reaction mediums and conditions for producing high yield of valuable monomers from concentrated sulfuric acid hydrolysed lignin. The solvent, temperature and time effects on the hydrogenolysis of hydrolysed lignin were investigated under the catalysis of Pd/C and $CrCl_3$. Supercritical methanol exhibits the best depolymerization performance, because of its unique diffusion, dissolution and acid–base properties. Afterwards, the influence of reaction temperature and time on depolymerization, repolymerization and coking during hydrogenolysis was examined in methanol. The high temperature is found to favour the depolymerization, with the β-O-4 linkages cleaved significantly. However, the repolymerization is promoted simultaneously, and a high amount of β-β groups form. These reactions are in constant competition with each other and the repolymerization is preferred at excessive high temperature, producing bulk char residues, that is coking. This study will provide a beneficial reference for the maximization of lignin waste valorization.

17/02072 Integrated utilization of algal biomass and corn stover for biofuel production

Yue, Z. *et al. Fuel*, 2016, 168, 1–6.
This paper describes a novel route for the utilization of algal and lignocellulosic biomass for biofuel production. Dilute sulfuric acid treatment was employed to destroy the rigid algal cells and generate algal hydrolysate. Algal hydrolysate was used as the reaction medium for the enzymatic hydrolysis of lignocellulose from corn stover. The acid treatment parameters were optimized based on the enzymatic efficiency of corn stover digestion and the promotion mechanism is discussed. The algal residues from the acid treatment process were co-digested with corn stover to generate methane. This study showed that algal hydrolysate can be used as a supplemental feedstock and reaction medium to enhance ethanol production. Furthermore, the residues could be utilized as the nitrogen source during the anaerobic digestion of corn stover.

17/02073 Isolation of lignin by organosolv process from different varieties of rice husk: Understanding their physical and chemical properties

Singh, S. K. and Dhepe, P. L. *Bioresource Technology*, 2016, 221, 310–317.
The aim of this work was to study the difference in properties of lignins, those (organosolv lignins (ORGLs, $12 \pm 3\%$ yield and $93 \pm 5\%$ mass balance) were isolated from diverse rice husk (RH) substrates using organosolv procedure (water : ethanol, H_2SO_4) carried out at 180 °C for 1 h. To identify the possible alterations in lignin structures several bulk and molecular level advanced characterization tools were employed. Even though lignins were extracted using common isolation procedure from three varieties of similar species of RH; from XRD, GPC, and elemental analysis it was found that those have comparable properties on bulk level. But molecular level analysis conducted using UV–vis, ATR, 1D/2D HSQC NMR techniques could help disclose that isolated lignins have varying concentrations of *G*, *H*, *S* and *T* substructures. Additionally, the double bond equivalence of 4.4–4.7 reveals that few of the aromatic rings are devoid of substituent.

17/02074 Microalgal biomass generation by phycoremediation of dairy industry wastewater: an integrated approach towards sustainable biofuel production

Chokshi, K. *et al. Bioresource Technology*, 2016, 221, 455–460.
Dairy wastewater collected from local dairy industry was used as a growth media (without any pre-treatment) for the cultivation of microalgae *Acutodesmus dimorphus*. The level of chemical oxygen demand reduced over 90% (from 2593.33 ± 277.37 to 215 ± 7.07 mg/L) after 4 days of cultivation; whereas, ammoniacal nitrogen was consumed completely (277.4 ± 10.75 mg/L) after 6 days of cultivation. Dry biomass of 840 and 790 mg/L was observed after 4 and 8 days of cultivation, respectively, which is about five or six times more than that of BG-11 grown culture (149 mg/L after 8 days). This biomass contains around 25% lipid and 30% carbohydrate, which can be further converted into biodiesel and bioethanol, respectively. Theoretical calculations based on the recently reported conversion yield suggest that 1 kg biomass of *A. dimorphus* might produce around 195 g of biodiesel and 78 g of bioethanol, which sums up to 273 g of biofuels.

17/02075 Microalgal cultivation with biogas slurry for biofuel production

Zhu, L. *et al. Bioresource Technology*, 2016, 220, 629–636.

Microalgal growth requires a substantial amount of chemical fertilizers. An alternative to the utilization of fertilizer is to apply biogas slurry produced through anaerobic digestion to cultivate microalgae for the production of biofuels. Plenty of studies have suggested that anaerobic digestate containing high nutrient contents is a potentially feasible nutrient source to culture microalgae. However, current literature indicates a lack of review available regarding microalgal cultivation with biogas slurry for the production of biofuels. To help fill this gap, this review highlights the integration of digestate nutrient management with microalgal production. It first unveils the current status of microalgal production, providing basic background to the topic. Subsequently, microalgal cultivation technologies using biogas slurry are discussed in detail. A scale-up scheme for simultaneous biogas upgrade and digestate application through microalgal cultivation is then proposed. Afterwards, several uncertainties that might affect this practice are explored. Finally, concluding remarks are put forward.

17/02076 Microbial community analysis using MiSeq sequencing in a novel configuration fluidized bed reactor for effective denitrification

Rungkitwatananukul, P. *et al. Bioresource Technology*, 2016, 221, 677–681.

A novel configured fluidized bed reactor (FBR) with granular rubber as the fluidized media was operated without internal recirculation to achieve denitrification. This FBR could operate under a low hydraulic retention time (HRT) of 50 min due to the low rubber media density and absence of recirculation. Synthetic nitrate-rich wastewater with a fixed nitrate (NO_3^--N) concentration and varying chemical oxygen demand (COD) concentrations was fed into the FBR. The nitrate removal profile showed a rapid nitrate reduction at the bottom of the reactor with a high performance under the low HRT. Different microbial communities were identified using Illumina Miseq sequencing. The dominant microorganisms belonged to the *Beta-* and *Gammaproteobacteria* classes and played important roles in nitrate reduction. *Acidovorax* was abundant at low $COD:NO_3^-$-N ratios, while *Rhizobium* and *Zoogloea* were dominant at high $COD:NO_3^-$-N ratios. The $COD:NO_3^-$-N ratio strongly influenced the composition of the microbial community including the dominant species.

17/02077 Monitoring sugar release during pipeline hydro-transport of wheat straw

Ghatora, S. *et al. Biomass and Bioenergy*, 2016, 93, 144–149.

Pipeline transport of biomass is an economically viable and technically feasible approach to replace conventional truck delivery approach and make the biomass-based energy industry more competitive with fossil fuel-based plants. A 25 m long and 50 mm diameter closed-circuit pipeline facility was fabricated to experimentally investigate the mechanical and chemical feasibility of transporting agricultural residue biomass–water mixtures (slurries) through pipelines. This research used the pipeline facility to study the loss of sugars (glucose and xylose) while pipelining wheat straw-water mixtures. The release of similar sugars was also measured in shake-flask cultures under controlled conditions. The output of this research is important for bio-processing facilities as a high sugar content slurry would improve the yield of biofuels produced from pipelined lignocellulosic materials. After several hours of recirculating throughout the pipeline, as well as shaking in the flask, a drop in sugar concentration was detected. A microbiological analysis performed on both slurries proved the decline to be due to microbial proliferation. Accordingly, diethyl pyrocarbonate oxidizing antimicrobial agent and glutaraldehyde and bronopol non-oxidizing agents were alternatively tested to restrict microbial proliferation. These agents demonstrated reduced sugar loss and, in turn, showed an enhancement in the yield of glucose and xylose. This research aims at maximizing possible sugar release through mechanical action throughout the pipeline in the presence of antimicrobial compounds, which would increase the yield of biofuel produced from pipelined agricultural residue biomass.

17/02078 Multivariate statistical process control charts for batch monitoring of transesterification reactions for biodiesel production based on near-infrared spectroscopy

Sales, R. F. *et al. Computers & Chemical Engineering*, 2016, 94, 343–353.

This work describes an application of multivariate statistical process control to monitor soybean oil transesterification. For the development of multivariate control charts, near infrared spectra were acquired in-line during the evolution of ten batches under normal operating conditions. They were then organized in a three-way array (batch × spectral variable × time). This structure was analysed by the two most commonly used approaches to develop batch monitoring schemes for handling such kind of data, referred to as Nomikos–MacGregor (NM) and Wold–Kettaneh–Friden–Holmberg (WKFH), respectively. To assess the performance of the approaches, eight test batches, during which specific interferences were induced, were manufactured. When applied for off-line monitoring, both NM and WKFH correctly pointed out such intentionally produced failures. On the other hand, concerning on-line monitoring, NM exhibited a better fault detection capability than WKFH. Contribution plots were found to highlight the spectral region mostly affected by the disturbances regardless of the modelling strategy resorted to.

17/02079 Nonlinear control of the dissolved oxygen concentration integrated with a biomass estimator for production of *Bacillus thuringiensis* δ-endotoxins

Rómoli, S. *et al. Computers & Chemical Engineering*, 2016, 93, 13–24.

Bacillus thuringiensis is a microorganism that allows the biosynthesis of δ-endotoxins with toxic properties against some insect larvae, being often used for the production of biological insecticides. A key issue for the bioprocess design consists in adequately tracking a pre-specified optimal profile of the dissolved oxygen concentration. To this effect, this paper aims at developing a novel control law based on a non-linear dynamic inversion method. The closed-loop strategy includes an observer based on a Bayesian regression with Gaussian process, which is used for on-line estimating the biomass present in the bioreactor. Unlike other approaches, the proposed controller leads to an improved response time with effective disturbance rejection properties, while simultaneously prevents undesired oscillations of the dissolved oxygen concentration. Simulation results based on available experimental data were used to show the effectiveness of the proposal.

17/02080 Quantitative characterization of the aqueous fraction from hydrothermal liquefaction of algae

Maddi, B. *et al. Biomass and Bioenergy*, 2016, 93, 122–130.

The aqueous fraction generated from hydrothermal liquefaction (HTL) of algae contains approximately 20–35% of the total carbon present in the algal feed. Hence, this aqueous fraction can be utilized to produce liquid fuels and/or specialty chemicals for economic sustainability of HTL on an industrial scale. In this study, aqueous fractions produced from HTL of freshwater and saline-water algal cultures were analysed using a wide variety of analytical instruments to determine their compositional characteristics. Organic chemical compounds present in eight aqueous fractions were identified using two-dimensional gas chromatography equipped with time-of-flight mass spectrometry. Identified compounds include organic acids, nitrogen compounds and aldehydes/ketones. Conventional gas chromatography and liquid chromatography methods were utilized to quantify the identified compounds. Inorganic species in the aqueous stream from HTL of algae also were quantified using ion chromatography and inductively coupled plasma optical emission spectroscopy. The concentrations of organic chemical compounds and inorganic species are reported. The amount quantified carbon ranged from 45% to 72% of the total carbon in the aqueous fractions.

17/02081 Re-thinking China's densified biomass fuel policies: large or small scale?

Shan, M. *et al. Energy Policy*, 2016, 93, 119–126.

Current policies and strategies related to the utilization of densified biomass fuel (DBF) in China are mainly focused on medium- or large-scale manufacturing modes, which cannot provide feasible solutions to solve the household energy problems in China's rural areas. To simplify commercial processes related to the collection of DBF feedstock and the production and utilization of fuel, a novel village-scale DBF approach is proposed. Pilot demonstration projects have shown the feasibility and flexibility of this new approach in realizing sustainable development in rural China. Effective utilization of DBF in rural China will lead to gains for global, regional, and local energy savings, environmental protection, sustainable development, and related social benefits. It could also benefit other developing countries for better utilization of biomass as a viable household energy source. This proposal therefore delivers the possibility of reciprocal gains, and as such deserves the attention of policy makers and various stakeholders.

17/02082 Simulated biogas oxidative reforming in AC-pulsed gliding arc discharge

Liu, J.-L. *et al. Chemical Engineering Journal*, 2016, 285, 243–251.

High-efficient oxidative reforming of simulated biogas in a novel AC-pulsed tornado gliding arc discharge was performed. The effects of two important factors, O_2/CH_4 ratio and specific energy input (*SEI*), were studied. Increasing the O_2/CH_4 ratio positively affected the reactant conversion, dry-basis concentration, and energy cost of syngas over the tested range of O_2/CH_4 ratios. Increasing the *SEI* increased the reactant conversion and dry-basis concentration of syngas but significantly increased the energy cost as well. Remarkable CO_2 conversion 25% (27%) and high dry-basis concentration of syngas 36% (71%) with a low energy cost of 66 kJ/mol (32 kJ/mol) were achieved for simulated biogas reforming with air (pure O_2) in this novel gliding arc reactor. In addition, in the oxidative reforming of simulated

biogas, syngas production was shown to be largely attributed to the partial oxidation reaction, and the remarkable CO_2 conversion was solely attributed to the reverse water gas shift reaction.

17/02083 Simulation of biomass-steam gasification in fluidized bed reactors: model setup, comparisons and preliminary predictions

Yan, L. *et al. Bioresource Technology*, 2016, 221, 625–635.

A user-defined solver integrating the solid-gas surface reactions and the multi-phase particle-in-cell (MP-PIC) approach is built based on the OpenFOAM software. The solver is tested against experiments. Then, biomass-steam gasification in a dual fluidized bed (DFB) gasifier is preliminarily predicted. It is found that the predictions agree well with the experimental results. The bed material circulation loop in the DFB can form automatically and the bed height is about 1 m. The voidage gradually increases along the height of the bed zone in the bubbling fluidized bed (BFB) of the DFB. The U-bend and cyclone can separate the syngas in the BFB and the flue gas in the circulating fluidized bed. The concentration of the gasification products is relatively higher in the conical transition section, and the dry and nitrogen-free syngas at the BFB outlet is predicted to be composed of 55% H_2, 20% CO, 20% CO_2 and 5% CH_4.

17/02084 Simultaneous hydrolysis and co-fermentation of whey lactose with wheat for ethanol production

Jin, Y. *et al. Bioresource Technology*, 2016, 221, 616–624.

Whey permeate was used as a co-substrate to replace part of the wheat for ethanol production by *Saccharomyces cerevisiae*. The simultaneous saccharification and fermentation was achieved with β-galactosidase added at the onset of the fermentation to promote whey lactose hydrolysis. *Aspergillus oryzae* and *Kluyveromyces lactis* β-galactosidases were two enzymes selected and used in the co-fermentation of wheat and whey permeate for the comparison of their effectiveness on lactose hydrolysis. The possibility of co-fermentations in both STARGEN and jet cooking systems was investigated in 5 L bioreactors. Ethanol yields from the co-fermentations of wheat and whey permeate were evaluated. It was found that *A. oryzae* β-galactosidase was more efficient for lactose hydrolysis during the co-fermentation and that whey permeate supplementation can contribute to ethanol yield in co-fermentations with wheat.

17/02085 Storage of whole-tree chips from high-density energy plantations of *Eucalyptus* in Brazil

de Jesus Eufrade Junior, H. *et al. Biomass and Bioenergy*, 2016, 93, 279–283.

In this paper, the drying of whole-tree chip (WTC) storage from a young Eucalyptus plantation managed at short-rotation coppice in Brazil was studied. The biomass was converted from high-density energy plantations of *Eucalyptus grandis* at 2 years old into four piles. Wood chip particles had 5, 15 and 30 mm length were disposed on a paved surface to evaluate the effect on the chip drying. An additional covered pile (30-mm wood chip) was installed to evaluate the effect of coverage condition. The non-ventilated and uncovered piles were not affected by WTC length, and the final moisture content (MC) was 48.4–53.5% and temperature inside the piles (storage temperature) was approximately 36 °C. However, the coverage showed beneficial effect on drying wood chip process, collaborating to keep the MC lower than 35%, conventionally recommended for energy purposes. Among storage systems studied, the higher daily moisture content was assigned to covered pile, about 0.197% day^{-1} during the first 30 days. This paper can be used as a reference for further studies with wood chip pile storage at tropical conditions.

17/02086 Sustainable production of bioethanol from renewable brown algae biomass

Lee, O. K. and Lee, E. Y. *Biomass and Bioenergy*, 2016, 92, 70–75.

Brown algae have been considered as renewable biomass for bioethanol production because of high growth rate and sugar level. Saccharification of brown algae biomass is relatively easy due to the absence of lignin. Among the major sugar components of brown algae, alginate cannot be directly used because industrial microorganisms are not able to metabolize alginate. This problem has been overcome by the development of metabolically engineered microbes to efficiently utilize alginate. This review analyses and evaluates recent research activities related to bioethanol production from brown algae. This review mainly deals with the recent development and potential of a metabolically engineered microbial cell factory and bioethanol production from brown algae biomass including alginate as the main carbohydrate. Future researches for cost-effective bioethanol production from brown algae are discussed.

17/02087 Thermal modelling of photovoltaic thermal (PVT) integrated greenhouse system for biogas heating

Tiwari, S. *et al. Solar Energy*, 2016, 136, 639–649.

In this paper, the design and fabrication of photovoltaic thermal integrated greenhouse system (PVTIGS) for biogas heating has been done for climatic condition of IIT Delhi, India. PVTIGS can also be used for a number of applications like generating electricity, space heating, enhancing production of biogas, crop cultivation and crop drying, etc. Thermal modelling of proposed system (PVTIGS) without load has been developed based on energy balance equations. Further, with the help of thermal modelling the solar cell temperature, room temperature and solar cell efficiency have been calculated for a typical clear day of May. Experimental validation have been done on the basis of correlation coefficient (r) and root mean square percentage deviation (e) and found to be in fair agreement between theoretical and experimental values. Effect of packing factor, mass flow rate of air below module, absorptivity (degradation effect) and transmittivity (dusting effect) on thermal load levelling have been discussed. Electrical energy has been calculated and validated with experimental values. Further, thermal energy and overall thermal energy have been evaluated and found to be 11.18 and 12.76 kW h, respectively, for a clear day without load.

17/02088 Thermochemical and physical evaluation of poplar genotypes as short rotation forestry crops for energy use

Monedero, E. *et al. Energy Conversion and Management*, 2016, 129, 131–139.

Short rotation plantations of fast-growing species provide a promising way to produce heat and electricity from renewable sources. The thermo-chemical and physical properties of different genotypes of poplar in short rotation forestry crops grown at three locations with different climatic and edaphic characteristics as well as planting density, have been determined in order to characterize the most appropriate biomass in terms of energy potential. The planting density was 6666 or 13,333 trees/ha (depending on the location) in a rotation of 3–4 years and the analysis was carried out at the end of the first rotation. For all the genotypes, experimental tests to quantify the moisture content, particle size distribution, bulk density, heating value, ash content and composition as well as the volatile matter were performed. In addition, natural air drying of biomass (stem and branches) was studied in two locations with the aim of determining the humidity loss during raw storage. A significant effect of the genotype and the planting density on the biomass properties was observed. The results obtained indicate that 'Monviso' and 'Viriato' are the most suitable genotypes. No operational problems related to ash fouling and deposition in combustion devices are expected for any of the genotypes studied.

17/02089 Use of laboratory anaerobic digesters to simulate the increase of treatment rate in full-scale high nitrogen content sewage sludge and co-digestion biogas plants

Tampio, E. *et al. Bioresource Technology*, 2016, 220, 47–54.

The aim of this study was to assess the effect of increasing feedstock treatment rate on the performance of full-scale anaerobic digestion using laboratory-scale reactors with digestate and feedstock from full-scale digesters. The studied nitrogen-containing feedstocks were (i) a mixture of industrial by-products and pig slurry and (ii) municipal sewage sludge, which digestion was studied at 41 and 52 °C, respectively. This study showed the successful reduction of hydraulic retention times from 25 and 20 days to around 15 days, which increased organic loading rates from 2 to 3.5 kg volatile solids (VS)/m^3 d and 4 to 6 kg VS/m^3 d. As a result, the optimum retention time in terms of methane production and VS removal was 10–15% lower than the initial in the full-scale digesters. Accumulation of acids during start-up of the co-digestion reactor was suggested to be connected to the high ammonium nitrogen concentration and intermediate temperature of 41 °C.

17/02090 Willingness of Kansas farm managers to produce alternative cellulosic biofuel feedstocks: an analysis of adoption and initial acreage allocation

Lynes, M. K. *et al. Energy Economics*, 2016, 59, 336–348.

This paper examines the likelihood that farm managers would be willing to harvest crop residue, or grow a dedicated annual or perennial bioenergy crop. In addition, factors affecting how many initial acres adopters would be willing to plant of a dedicated annual or perennial bioenergy crop are assessed. The study finds several factors affect farm managers' decisions to harvest crop residue, or grow annual or perennial bioenergy crops, as well as their potential initial acreage allocation decisions. These factors lead to several policy implications that should be tailored to the specific type of cellulosic bioenergy crop.

17/02091 WO_x modified Cu/Al_2O_3 as a high-performance catalyst for the hydrogenolysis of glucose to 1,2-propanediol

Liu, C. *et al. Catalysis Today*, 2016, 261, 116–127.

Glucose is one of the most important platform molecules of biomass in nature. The selective hydrogenolysis of glucose to 1,2-PDO is still a challenge. However, The hydrogenolysis of fructose has higher activity and selectivity to 1,2-PDO. Therefore, A series of Cu-WO_x/Al_2O_3 catalysts with high activity for glucose isomerization to fructose and fructose hydrogenolysis to 1,2-PDO were designed for glucose hydrogenolysis to 1,2-PDO. The W surface density was controlled as low as 0.8 W/nm^2. The low W surface density could make the WO_x species present as isolated WO_4 structure, which could only provide more Lewis acid sites. As a result, the isolated WO_4 species could form a complex with glucose and then promote the isomerization of glucose to fructose. The isolated WO_4 species also have coverage, dispersion, and electronic effects on copper sites, resulting more stable copper sites and proper amount of hydrogenation sites on Cu-WO_x/Al_2O_3 surface. The correlations between the ratio of Lewis acid amount to Cu surface area and the selectivity of 1,2-PDO suggest that the hydrogenolysis of glucose to 1,2-PDO follows the bifunctional reaction route which contains the reactions on Lewis acid and metal sites. Furthermore, the highest 1,2-PDO selectivity of 55.4% was obtained on Cu-WO_x(0.8)/Al_2O_3.

Geothermal energy

17/02092 Coupling short-term (B2G model) and long-term (g-function) models for ground source heat exchanger simulation in TRNSYS. Application in a real installation
Ruiz-Calvo, F. *et al. Applied Thermal Engineering*, 2016, 102, 720–732.
Ground-source heat pump (GSHP) systems represent one of the most promising techniques for heating and cooling in buildings. These systems use the ground as a heat source/sink, allowing a better efficiency thanks to the low variations of the ground temperature along the seasons. The ground-source heat exchanger (GSHE) then becomes a key component for optimizing the overall performance of the system. Moreover, the short-term response related to the dynamic behaviour of the GSHE is a crucial aspect, especially from a regulation criteria perspective in on/off controlled GSHP systems. In this context, a novel numerical GSHE model has been developed at the Instituto de Ingeniería Energética, Universitat Politècnica de València in Spain. Based on the decoupling of the short-term and the long-term response of the GSHE, the novel model allows the use of faster and more precise models on both sides. In particular, the short-term model considered is the B2G model, developed and validated in previous research works conducted at the Instituto de Ingeniería Energética. For the long-term, the g-function model was selected, since it is a previously validated and widely used model, and presents some interesting features that are useful for its combination with the B2G model. The aim of the present paper is to describe the procedure of combining these two models in order to obtain a unique complete GSHE model for both short- and long-term simulation. The resulting model is then validated against experimental data from a real GSHP installation.

17/02093 Early-flowback tracer signals for fracture characterization in an EGS developed in deep crystalline and sedimentary formations: a parametric study
Karmakar, S. *et al. Geothermics*, 2016, 63, 242–252.
Artificial-fracture design and fracture characterization is a central aspect of many enhanced geothermal system (EGS) projects. The use of single well (SW) short-term tracer signals to characterize fractures at the Groß-Schönebeck EGS pilot site is explored in this paper. A certain degree of parameter interdependence in short-term flowback signals leads to ambiguity in fracture parameter inversion from measured single-tracer signals. This ambiguity can, to some extent, be overcome by (a) combining different sources of information, and/or (b) using different types of tracers, such as conservative tracer pairs with different diffusivities, or tracer pairs with contrasting sorptivities on target surfaces. Fracture height is likely to be controlled by lithostratigraphy while fracture length can be determined from hydraulic monitoring (pressure signals). Since the flowback rate is known during an individual-fracture test, the unknown parameters to be inferred from tracer tests are (i) transport-effective aperture in a water fracture or (ii) fracture thickness and porosity for a gel-proppant fracture. Tracers with different sorptivity on proppant coatings and matrix rock surfaces for gel-proppant fractures, and tracers with contrasting-diffusivity or -sorptivity for a water fracture were considered. An advantage of this approach is that it requires only a very small chaser injection volume (about half of fracture volume).

17/02094 Exergoenvironmental and exergoeconomic analyses of a vertical type ground source heat pump integrated wall cooling system
Akbulut, U. *et al. Applied Thermal Engineering*, 2016, 102, 904–921.
In this study, exergoenvironmental, and exergoeconomic analyses of wall cooling systems fed by a vertical type of ground source heat pump integrated wall cooling system for cooling were examined experimentally and theoretically in the Yildiz renewable energy house at Davutpaşa Campus of Yildiz Technical University, Istanbul, Turkey. The examination includes energy, exergy, exergoenvironmental and exergoeconomic analyses, between the dates of 1 July and 30 September 2013. The main aim here was to minimize energy usage in the residential sector as much as possible. Therefore, a particular system working with low temperature regime was chosen. According to the outcomes; energy and exergy efficiency of all the system have been found as 74.85% and 29.90%. Part-based environmental factor values are calculated. The compressor and underground heat exchanger have the highest values calculated as 0.040 and 0.026 mPts/s respectively. The exergoenvironmental impact values of all system are detected as 42.60%. On the other hand; the exergoeconomic factor values of all system are calculated as 77.68%. The value of exergoeconomic factor changes depending on some particular components: accumulator tank, undersoil heat exchanger, evaporator and condenser calculated respectively as 69.43%, 62.59%, 62.53% and 29.15%. As a result; it is found that in order to determine economic and environmental impacts of irreversibilities occurring in the system and its components, economic and environmental analyses of thermal system as well as wall cooling systems, should be done based on exergy concept.

17/02095 Experimental investigation of a ground-coupled desiccant assisted air conditioning system
Speerforck, A. and Schmitz, G. *Applied Energy*, 2016, 181, 575–585.
In a pilot installation at Hamburg University of Technology the coupled operation of an open cycle desiccant assisted air conditioning system with borehole heat exchangers is investigated. The paper presents experimental data recorded during the cooling period 2014. Results show that the electricity demand of the system can be reduced to the parasitic consumption of the fans, wheels and pumps. An electric energy efficiency ratio of 6.63 is achieved, enabling electricity savings of more than 70% compared to a conventional reference system and 54% compared to a desiccant assisted hybrid system relying on an electric chiller. Comfort conditions can be maintained during the whole cooling period. The borehole heat exchangers work highly efficient, exhibiting a seasonal performance factor of 192.

17/02096 Experimental study of thermal performance of a ground source heat pump system installed in a Himalayan city of India for composite climatic conditions
Sivasakthivel, T. *et al. Energy and Buildings*, 2016, 131, 193–206.
Space heating and cooling appliances consume a significant amount of energy in buildings. In recent decades, ground source heat pump (GSHP) systems have become popular for space heating applications in many countries. However, countries like India need both space heating and cooling and hence its performance needs to be evaluated in both heating and cooling functions for economical operation. The experimental results obtained for both modes of operation are discussed in detail in this paper. Details of the experimental setup used, measurements, performance of ground heat exchanger (GHX) used and calculation of coefficient of performance (COP), effectiveness and extraction/injection are explained. Using the experimental data the COP of heat pump and GSHP are obtained. The average COP of the GSHP system obtained during space cooling was found to be 21% less than the value obtained for heating mode operation and also heat extraction by the GHX fluid is observed to be high at the starting of the operation. In heat injection mode, as the operational time increases, the surrounding soil temperature also increased thus creating more resistance for heat flow. The average effectiveness of GHX was found to be 0.29 and 0.33 in heating and cooling mode operations, respectively.

17/02097 Geothermal solute flux monitoring and the source and fate of solutes in the Snake River, Yellowstone National Park, WY
McCleskey, R. B. *et al. Applied Geochemistry*, 2016, 73, 142–156.
The combined geothermal discharge from over 10,000 features in Yellowstone National Park (YNP) can be can be estimated from the Cl flux in the Madison, Yellowstone, Falls, and Snake Rivers. Over the last 30 years, the Cl flux in YNP Rivers has been calculated using discharge measurements and Cl concentrations determined in discrete water samples and it has been determined that approximately 12% of the Cl flux exiting YNP is from the Snake River. The relationship between electrical conductivity and concentrations of Cl and other geothermal solutes was quantified at a monitoring site located downstream from the thermal inputs in the Snake River. Beginning in 2012, continuous (15 min) electrical conductivity measurements have been made at the monitoring site. Combining continuous electrical conductivity and discharge data, the Cl and other geothermal solute fluxes were determined. The 2013–2015 Cl fluxes (5.3–5.8 kt/yr) determined using electrical conductivity are comparable to historical

data. In addition, synoptic water samples and discharge data were obtained from sites along the Snake River under low-flow conditions of September 2014. The synoptic water study extended 17 km upstream from the monitoring site. Surface inflows were sampled to identify sources and to quantify solute loading. The Lewis River was the primary source of Cl, Na, K, Cl, SiO_2, Rb, and As loads (50–80%) in the Snake River. The largest source of SO_4 was from the upper Snake River (50%). Most of the Ca and Mg (50–55%) originate from the Snake Hot Springs. Chloride, Ca, Mg, Na, K, SiO_2, F, HCO_3, SO_4, B, Li, Rb, and As behave conservatively in the Snake River, and therefore correlate well with conductivity ($R^2 \geq 0.97$).

17/02098 Optimisation of experimental operation of borehole thermal energy storage

Rapantova, N. *et al. Applied Energy*, 2016, 181, 464–476.

Although a variety of engineering guidelines, planning software and modelling techniques are available for shallow geothermal system planning and design, only a few studies have investigated their long-term operational effects in the field. The present study deals with an *in situ* experiment on a borehole thermal energy storage (BTES) from combined heat and power production (CHP), which has been in operation on the site of Green Gas DPB in Paskov (the Czech Republic) for more than 3 years. This experimental BTES was monitored through six monitoring boreholes, and the temperatures were measured at various depths up to 80 m under the ground. The maximum temperatures measured at the centre of the BTES at the depths of 2–60 m under the ground ranged from 69.0 to 78.5 °C. The data acquired from the BTES operation were then used to set up and calibrate a heat transport model in the rock environment by means of the FEFLOW code. The calibrated numerical model contributed to optimization of the BTES operation by simulation of various cycles of injection and exploitation of heat with an objective to minimize the loss of heat due to dissipation to the ground. The long-term feasibility of 65% recovery of heat stored underground in the BTES in Paskov was predicted, and recommendations concerning efficient operation of this BTES were provided.

17/02099 Performance assessment of vortex tube and vertical ground heat exchanger in reducing fuel consumption of conventional pressure drop stations

Ghezelbash, R. *et al. Applied Thermal Engineering*, 2016, 102, 213–226.

In natural gas pressure drop stations, before pressure dropping specially in cold seasons, the natural gas is preheated to prevent gas hydrate formation. Indirect water bath heaters employed for preheating. The heaters have low thermal efficiency and consume a large amount of natural gas for preheating. Due to the abundance of natural gas pressure reduction stations, reducing energy consumption is essential in this sector of the gas industry. In this study to reduce the heater energy consumption, an innovative system based on using vortex tube and vertical ground heat exchanger is proposed. A vortex tube is used instead of throttle valve to reduce natural gas pressure. Unlike the throttle valve, vortex tube divides the incoming stream into two cold and hot streams. Cold stream enters the shell and tube heat exchanger and receives geothermal heat. Then the warmed cold stream mix with hot steam outgoing from the vortex tube, and goes towards the heater at low pressure. The proposed system can reduce energy consumption up to 88%, and the discounted payback period is always less than 4.5 years.

17/02100 Physical, chemical and mineralogical evolution of the Tolhuaca geothermal system, southern Andes, Chile: insights into the interplay between hydrothermal alteration and brittle deformation

Sanchez-Alfaro, P. *et al. Journal of Volcanology and Geothermal Research*, 2016, 324, 88–104.

This study unravels the physical, chemical and mineralogical evolution of the active Tolhuaca geothermal system in the Andes of southern Chile. The authors used temperature measurements in the deep wells and geochemical analyses of borehole fluid samples to constrain present-day fluid conditions. In addition, they reconstructed the paleo-fluid temperatures and chemistry from microthermometry and LA-ICP-MS analysis of fluid inclusions taken from well-constrained parageneses in vein samples retrieved from a ~1000 m borehole core. Based on core logging, mineralogical observations and fluid inclusions data, the authors identified four stages (S1–S4) of progressive hydrothermal alteration. An early heating event (S1) was followed by the formation of a clay-rich cap in the upper zone (<670 m) and the development of a propylitic alteration assemblage at greater depth (S2). Boiling, flashing and brecciation occurred later (S3), followed by a final phase of fluid mixing and boiling (S4). The evolution of hydrothermal alteration at Tolhuaca has produced a mineralogical, hydrological and structural vertical segmentation of the system through the development of a low-permeability, low-cohesion clay-rich cap at shallow depth. The quantitative chemical analyses of fluid inclusions and borehole fluids reveal a significant change in chemical conditions during the evolution of Tolhuaca. Whereas borehole (present-day) fluids are rich in Au, B and As, but Cu-poor ($B/Na \sim 10^{0.5}$, $As/Na \sim 10^{-1.1}$, $Cu/Na \sim 10^{-4.2}$), the paleofluids trapped in fluid inclusions are Cu-rich but poor in B and As ($B/Na \sim 10^{-1}$, $As/Na \sim 10^{-2.5}$, $Cu/Na \sim 10^{-2.5}$ in average). The fluctuations in fluid chemistry at Tolhuaca were interpreted as the result of transient supply of metal-rich, magmatically derived fluids where As, Au and Cu are geochemically decoupled. Since these fluctuating physical and chemical conditions at the reservoir produced a mineralogical vertical segmentation of the system that affects the mechanical and hydrological properties of host rock, the authors explored the effect of the development of a low-cohesion low-permeability clay cap on the conditions of fault rupture and on the long-term thermal structure of the system. These analyses were performed by using rock failure condition calculations and numerical simulations of heat and fluid flows. Calculations of the critical fluid pressures required to produce brittle rupture indicate that within the clay-rich cap, the creation or reactivation of highly permeable extensional fractures is inhibited. In contrast, in the deep upflow zone the less pervasive formation of clay mineral assemblages has allowed retention of rock strength and dilatant behaviour during slip, sustaining high permeability conditions. Numerical simulations of heat and fluid flows support the observations and suggest that the presence of a low permeability clay cap has helped increase the duration of high-enthalpy conditions by a factor of three in the deep upflow zone at Tolhuaca geothermal system, when compared with an evolutionary scenario where a clay cap was not developed. Furthermore, the data demonstrate that the dynamic interplay between fluid flow, crack-seal processes and hydrothermal alteration are key factors in the evolution of the hydrothermal system, leading to the development of a high enthalpy reservoir at the flank of the dormant Tolhuaca volcano.

17/02101 Resistivity structure and geochemistry of the Jigokudani Valley hydrothermal system, Mt. Tateyama, Japan

Seki, K. *et al. Journal of Volcanology and Geothermal Research*, 2016, 325, 15–26.

This study clarifies the hydrothermal system of Jigokudani Valley near Mt. Tateyama volcano in Japan by using a combination of audio-frequency magnetotelluric (AMT) survey and hot-spring water analysis in order to assess the potential of future phreatic eruptions in the area. Repeated phreatic eruptions in the area about 40,000 years ago produced the current valley morphology, which is now an active solfatara field dotted with hot springs and fumaroles indicative of a well-developed hydrothermal system. The three-dimensional (3D) resistivity structure of the hydrothermal system was modelled by using the results of an AMT survey conducted at 25 locations across the valley in 2013–2014. The model suggests the presence of a near-surface highly conductive layer of <50 m in thickness across the entire valley, which is interpreted as a cap rock layer. Immediately below the cap rock is a relatively resistive body interpreted as a gas reservoir. Field measurements of temperature, pH, and electrical conductivity (EC) were taken at various hot springs across the valley, and 12 samples of hot-spring waters were analysed for major ion chemistry and H_2O isotopic ratios. All hot-spring waters had low pH and could be categorized into three types on the basis of the Cl^-/SO_4^{2-} concentration ratio, with all falling largely on a mixing line between magmatic fluids and local meteoric water). The geochemical analysis suggests that the hydrothermal system includes a two-phase zone of vapour–liquid. A comparison of the resistivity structure and the geochemically inferred structure suggests that a hydrothermal reservoir is present at a depth of approximately 500 m, from which hot-spring water differentiates into the three observed types. The two-phase zone appears to be located immediately beneath the cap rock structure. These findings suggest that the hydrothermal system of Jigokudani Valley exhibits a number of factors that could trigger a future phreatic eruption.

17/02102 Temperature response factors at different boundary conditions for modelling the single borehole heat exchanger

Priarone, A. and Fossa, M. *Applied Thermal Engineering*, 2016, 103, 934–944.

Design and simulation of borehole heat exchangers rely on the solution of the transient conduction equation. The typical approach for predicting the ground temperature variations in the short and long term is to recursively apply basic thermal response factors available as analytical functions or as pre-estimated tabulated values. In this paper a review of the existing response factor models for borehole heat exchangers (BHE) analysis is presented and a numerical model, built in Comsol environment is employed for calculating the temperature distribution in time and space around a single, finite length, vertical cylindrical heat source also taking into account its position with reference to the ground surface (effects of the adiabatic length or 'buried depth' D). The temperature values are recast as dimensionless response factors in order to compare them with analytical solutions

where available. Furthermore new temperature response factors suitable for describing the single finite cylindrical source (FCS) under different operating modes (i.e. boundary conditions) are generated. Boundary conditions include imposed heat transfer rate, imposed temperature and a combination of both conditions, where spatially uniform temperature at the BHE interface is attained while also keeping constant the applied heat transfer rate.

17/02103 Thermo-poroelastic effects on reservoir seismicity and permeability change

Ghassemi, A. and Tao, Q. *Geothermics*, 2016, 63, 210–224.

This study considers the role of thermo-poromechanical processes on reservoir seismicity and permeability enhancement using theoretical/numerical analysis. The numerical model is fully coupled, considering non-isothermal compressible single-phase fluid flow in fractured porous rock. It combines the thermo-poroelastic displacement discontinuity method, a non-linear joint deformation model, and a finite difference method for solving the fluid and heat transport in a fracture network. The model is applied to simulate cool water injection into fracture/matrix systems to examine the role of coupled processes on fracture deformation, matrix pore pressure and stress redistributions to assess their role in induced seismicity and permeability variations. The simulation results are analysed to draw conclusions regarding injection rate dependence of seismicity, and its transience due to coupled processes. Thermal influence on pore pressure and stress tend to promote delayed seismicity. In presence of coupled processes, rock matrix stress perturbations due to natural fracture deformation can be an influencing mechanism for seismicity. The results show the induced normal stress in the vicinity of the fracture centre where injected water enters, can be significant for higher cooling levels in low permeability matrix, and induces additional pore pressure perturbations in the matrix. These couplings have implications for reservoir stimulation and induced seismicity in geothermal reservoirs. The reservoir rock can experience a series of induced stress/pore pressure regimes with continued cooling (under injection). A potentially destabilizing regime is followed by a stabilizing one, and subsequently the rock approaches a destabilizing state. Each situation can result in potentially different levels of MEQ activity. Finally, the impact of thermo-poroelastic stresses on injection/extraction pressure profiles in a fractured rock is illustrated. Injection pressure tends to initially increase in response to poroelastic stress, but with time the thermal effect dominates resulting in fracture aperture increases and lowering of injection pressure.

Solar energy

17/02104 A new backstepping finite time sliding mode control of grid connected PV system using multivariable dynamic VSC model

Dhar, S. and Dash, P. K. *International Journal of Electrical Power & Energy Systems*, 2016, 82, 314–330.

This paper presents independent active and reactive power management of a three-phase grid-connected photovoltaic (PV) generation system using a new non-linear control approach for the voltage source converter (VSC). Instead of controlling the direct and quadrature-axis currents of the VSC, the instantaneous active and reactive powers are used as error estimation parameters. This mode of control dispenses the unmodelled dynamics of the VSC phase-locked loop system and produces a robust control for the active–reactive power, and dc voltage excursions. This approach reduces computational time as well as complexity by avoiding unnecessary phase-locked loop (PLL) phase calculation in the beginning. However, the PLL is used only to obtain the frequency component needed to generate the PWM signal. Further to improve the stability and robust tracking of the grid connected PV array, backstepping finite time fast sliding mode (BFTSM) control strategy is presented in this paper. The proposed controller offers invariant stability to modelling uncertainties due to converter parameter changes, changes in system frequency and exogenous inputs. Also the finite time sliding mode control offers an important tool for designing continuous finite time control laws. Comprehensive computer simulations are carried out in MATLAB/Simulink to verify the proposed control scheme under several system disturbances like changes in solar insolation, changes in local load, converter parametric changes, and faults on the converter and inverter buses, and partial shading condition of PV array. EMTDC/PSCAD model is established as confirmative study.

17/02105 An open-source optimization tool for solar home systems: a case study in Namibia

Campana, P. E. *et al. Energy Conversion and Management*, 2016, 130, 106–118.

Solar home systems (SHSs) represent a viable technical solution for providing electricity to households and improving standard of living conditions in areas not reached by the national grid or local grids. For this reason, several rural electrification programmes in developing countries, including Namibia, have been relying on SHSs to electrify rural off-grid communities. However, the limited technical know-how of service providers, often resulting in over- or under-sized SHSs, is an issue that has to be solved to avoid dissatisfaction of SHSs' users. The solution presented here is to develop an open-source software that service providers can use to optimally design SHSs components based on the specific electricity requirements of the end-user. The aim of this study is to develop and validate an optimization model written in MS Excel-VBA which calculates the optimal SHSs components capacities guaranteeing the minimum costs and the maximum system reliability. The results obtained with the developed tool showed good agreement with a commercial software and a computational code used in research activities. When applying the developed optimization tool to existing systems, the results identified that several components were incorrectly sized. The tool has thus the potentials of improving future SHSs installations, contributing to increasing satisfaction of end-users.

17/02106 Carbon-based two-dimensional layered materials for photocatalytic CO_2 reduction to solar fuels

Low, J. *et al. Energy Storage Materials*, 2016, 3, 24–35.

The depletion of fossil fuels and rising atmospheric levels of carbon dioxide lead to an increasing interest in artificial photosynthesis technologies. Among them, photocatalytic CO_2 reduction to valuable solar fuels is considered as one of the best strategies for solving both energy and environmental problems simultaneously. In the past decade, it was proved that the photocatalytic CO_2 reduction performance can be greatly enhanced by using carbon-based two-dimensional (2D) layered materials, namely graphene and graphitic carbon nitride ($g\text{-}C_3N_4$) due to their excellent electronic and physicochemical properties. In this review, the major advances in the area of carbon-based 2D layered photocatalysts for CO_2 reduction are presented. A brief overview on the preparation methods and applications of carbon-based 2D layered photocatalysts is discussed. Finally, the challenges and opportunities for the future research of carbon-based 2D layered materials in photocatalytic CO_2 reduction are highlighted.

17/02107 Combined probation of bubble column humidification dehumidification desalination system using solar collectors

Rajaseenivasan, T. *et al. Energy*, 2016, 116, 459–469.

A bubble column (BC) humidification dehumidification (HDH) desalination system integrated with the different solar collectors is analysed and reported in this work. Major components of the systems are a humidifier, dehumidifier, solar air heater (SAH), and dual purpose collector (DPC). Three set of experiments is performed by integrating the HDH system with conventional solar air heater (case I), by integrating with solar air heater containing turbulators (case II), and by integrating with dual purpose solar collector containing turbulators (case III). Turbulators in the air flow field of solar collector enhances the exit air temperature. The air and water are simultaneously heated up in the dual purpose collector and supplied to the humidifier. All the experiments are done by varying the mass flow rate of air (0.014–0.018 kg/s) and cooling water (0.025–0.058 kg/s). The performance of the system is improved with the increase in air and cooling water flow rate. Gained output ratios of about 2, 2.8, 3.3 and productivities of around 16.32, 20.61, 23.92 kg/m^2 day are observed in cases I, II and III, respectively. The minimum distilled water cost of \$0.019/kg is achieved with the case III configuration.

17/02108 Counter electrodes from polymorphic platinum-nickel hollow alloys for high-efficiency dye-sensitized solar cells

Wang, J. *et al. Journal of Power Sources*, 2016, 328, 185–194.

Precious platinum counter electrodes (CE) have been an economic burden for the future commercialization of dye-sensitized solar cells (DSSCs). Low-platinum alloy CE catalysts are promising in bringing down the solar cell cost without reducing photovoltaic performances. This study presents a facile strategy of fabricating ZnO nanorods assisted platinum-nickel (PtNi) alloy microtube CEs for liquid-junction DSSCs. By adjusting the concentration of zinc precursors, the ZnO nanostructures and therefore PtNi alloys are optimized to maximize the electrocatalytic behaviours toward triiodide reduction reaction. The maximal power conversion efficiency is determined as high as 8.43% for liquid-junction DSSC device with alloyed PtNi microtube CE synthesized at 75 mM $Zn(NO_3)_2$ aqueous solution, yielding a 32.8% enhancement in cell efficiency in comparison with the solar cell from pristine platinum electrode. Moreover, the dissolution resistance and charge-transfer ability toward redox couples have also been markedly enhanced due to competitive dissolution reactions and alloyed effects.

17/02109 Design and optical analysis of the band-focus Fresnel lens solar concentrator

Wang, G. *et al. Applied Thermal Engineering*, 2016, 102, 695–700.

Solar energy is one of the most promising renewable energies and meaningful for the sustainable development of energy source. In this paper, a new kind of band-focus Fresnel lens solar concentrator was proposed. The design principle of this solar concentrator was given and the spectral concentrating performance was simulated by the means of Monte Carlo ray tracing method, which was compared with the linear Fresnel lens. The results show that both the spectral concentrating uniformity and optical efficiency of the band-focus Fresnel lens were better than those of the linear one. Meanwhile several characteristic parameters of the band-focus Fresnel lens concentrator were analysed under different conditions and it can be drawn from the results that a high-ratio band-focus Fresnel lens concentrator could increase the optical efficiency of a concentrating photovoltaic system.

17/02110 Design and real time implementation of a novel rule compressed fuzzy logic method for the determination operating point in a photo voltaic system

Rajesh, R. and Mabel, M. C. *Energy*, 2016, 116, 140–153.

In the photovoltaic (PV) system characteristics, a maximum power operating point exists for each value of solar irradiance. The operating point continuously varies as the solar irradiance vary and therefore tracking of maximum power in PV system is significant. This paper introduces a new rule compressed fuzzy logic method to track optimal power operating point of photovoltaic system under non-uniform irradiance. The method has three-input parameters and a single output parameter. The input parameters are the change in power, the change in voltage and change in duty cycle and the output parameter is the reference current to the converter. With respect to each combination of two input parameters, three set of output rules are developed and then compressed to a single set of rules based on tracking conditions. The step response, analysis under partial shading and with one day solar irradiance data are implemented in Matlab/Simulink platform. The method confirms its effectiveness by attaining the optimal power at 2.46 s with a low steady state error of 0.35%. The energy capitulation efficiency is obtained as 99.5%. The performance of the proposed method is also evaluated experimentally and its efficiency is proved by comparing with perturb and observe algorithm.

17/02111 Design of maintenance structures for rural electrification with solar home systems. The case of the Moroccan program

Carrasco, L. M. *et al. Energy*, 2016, 117, 47–57.

In decentralized rural electrification through solar home systems, private companies and promoting institutions are faced with the problem of deploying maintenance structures to operate and guarantee the service of the solar systems for long periods (10 years or more). The problems linked to decentralization, such as the dispersion of dwellings, difficult access and maintenance needs, makes it an arduous task. This paper proposes an innovative design tool created *ad hoc* for photovoltaic rural electrification based on a real photovoltaic rural electrification programme in Morocco as a special case study. The tool is developed from a mathematical model comprising a set of decision variables (location, transport, etc.) that must meet certain constraints and whose optimization criterion is the minimum cost of the operation and maintenance activity assuming an established quality of service. The main output of the model is the overall cost of the maintenance structure. The best location for the local maintenance headquarters and warehouses in a given region is established, as are the number of maintenance technicians and vehicles required.

17/02112 Detailed performance analysis of realistic solar photovoltaic systems at extensive climatic conditions

Gupta, A. and Chauhan, Y. K. *Energy*, 2016, 116, 716–734.

In recent years, solar energy has been considered as one of the principle renewable energy source for electric power generation. In this paper, single diode photovoltaic (PV) system and double/bypass diode-based PV system are designed in MATLAB/Simulink environment based on their mathematical modelling and are validated with a commercially available solar panel. The novelty of the paper is to include the effect of climatic conditions, i.e. variable irradiation level, wind speed, temperature, humidity level and dust accumulation in the modelling of both the PV systems to represent a realistic PV system. The comprehensive investigations are made on both the modelled PV systems. The obtained results show the satisfactory performance for realistic models of the PV system. Furthermore, an in depth comparative analysis is carried out for both PV systems.

17/02113 Dynamic simulation of a solar heating and cooling system for an office building located in southern Italy

Angrisani, G. *et al. Applied Thermal Engineering*, 2016, 103, 377–390.

The paper investigates the introduction of a solar heating and cooling system in an office building characterized by low energy demand with respect to the current national building stock and located in southern Italy. Dynamic simulations are carried out in order to evaluate the thermo-economic performance of the analysed system considering different solar panel technologies (flat plate and evacuated tube), tilt angles (10–70°), collecting areas (30–60 m^2), hot and cold storage sizes, reference emission factors, electricity and natural gas unitary prices. To satisfy cooling demand a small scale adsorption chiller activated by thermal energy available from solar collectors is considered. The solar heating and cooling system demonstrated primary energy saving and equivalent dioxide carbon emission reduction higher than 23% in comparison to the reference conventional system. The results show that the solar energy system will be competitive when the electricity and natural gas prices will be high and strong government incentives will be provided.

17/02114 Enhanced thermal energy supply via central solar heating plants with seasonal storage: a multi-objective optimization approach

Tulus, V. *et al. Applied Energy*, 2016, 181, 549–561.

Central solar heating plants with seasonal storage (CSHPSS) are among the most promising technologies to save energy in the industrial and residential–commercial building sectors. This work introduces a systematic approach to optimize these systems according to economic and environmental criteria. This method, which combines the TRNSYS 17 simulation software with life cycle assessment and multi-objective optimization, identifies optimal CSHPSS designs for any climatic condition and heating demand profile considering economic and environmental criteria simultaneously. The capabilities of this approach are illustrated through its application to a case study of a CSHPSS located in Barcelona, Spain, which satisfies a heating demand for a neighbourhood of 1120 dwellings. Numerical results show that the CSHPSS plant leads to significant environmental and economic improvements compared to the use of a conventional natural gas heating system. This tool can guide engineers and architects in the transition towards a more sustainable residential sector.

17/02115 Experimental and numerical investigation of a linear Fresnel solar collector with flat plate receiver

Bellos, E. *et al. Energy Conversion and Management*, 2016, 130, 44–59.

In this study a linear Fresnel solar collector with flat plate receiver is investigated experimentally and numerically with Solidworks Flow Simulation. The developed model combines optical, thermal and flow analysis; something innovative and demanding which leads to accurate results. The main objective of this study is to determine the thermal, the optical and the exergetic performance of this collector in various operating conditions. For these reasons, the developed model is validated with the respective experimental data and after this step, the solar collector model is examined parametrically for various fluid temperature levels and solar incident angles. The use of thermal oil is also analysed with the simulation tool in order to examine the collector performance in medium temperature levels. The experiments are performed with water as working fluid and for low temperature levels up to 100 °C. The final results proved that this solar collector is able to produce about 8.5 kW useful heat in summer, 5.3 kW in spring and 2.9 kW in winter. Moreover, the operation of this collector with thermal oil can lead to satisfying results up to 250 °C.

17/02116 Experimental performance evaluation and modeling of jet impingement cooling for thermal management of photovoltaics

Bahaidarah, H. M. S. *Solar Energy*, 2016, 135, 605–617.

Thermal management of photovoltaic (PV) systems is one of the most important factors that affect the overall performance especially in hot climate regions. In this paper, the viability of jet impingement cooling for PV panels subjected to the climatic conditions of Dhahran region of Middle East has been discussed. Experimental and numerical performance evaluation was carried out for two configurations, an uncooled PV system and an impingement cooled PV system. The complete cooling model incorporates optical, radiation, thermal, geometric and electrical model for the overall performance analysis of the PV system. Jet impingement geometric model for PV was developed to carry out the heat transfer analysis for single nozzle for analysing the cell temperature, power output and conversion efficiency of PV strings. For precise prediction of the performance of the PV cell, seven parameters electrical model is employed, whereas for absorbed radiation calculation isotropic sky model is adopted. Temperature measurements revealed cell temperature as high as 69.7 °C and 47.6 °C for an uncooled system for June and December, respectively. By applying jet cooling, average cell temperature was reduced to 36.6 °C for June and 31.1 °C for December. Power output and conversion efficiency was enhanced by 51.6% and 66.6% by employing jet cooling for June, respectively. Similarly, December results revealed performance improvement by 49.6% in power output and 82.6% in conversion

efficiency. Simulation carried out reveals that jet cooling with optimum parameters has not only significantly increased the electrical power output and cell efficiency but has reduced the cell temperature while keeping it uniform for each cell.

17/02117 Experimental thermal evaluation of a novel solar collector using magnetic nano-particles

Xu, G. *et al. Energy Conversion and Management*, 2016, 130, 252–259.
A novel solar thermal collector using magnetic nanoparticles to create a special array structure to capture solar light to enhance the thermal efficiency is put forward. The gradient-index optics theory is used to explain the physics of the proposed system. A set of experimental facility is set up to test the thermal collecting efficiency and a comparison between the coating vacuum tube and the conventional vacuum tube is conducted. The authors used 180 nm sphere iron nanoparticles under the stagnation experiment with water as the working medium. Results show that the magnetic tube performs as well as the coating tubes in lower temperatures and better than ordinary tubes all the time. Heat loss analysis shows the magnetic array structure has a larger ability to capture solar light while a lower ability to prevent heat loss due to the low emissivity layer in the coating. The normalized temperature difference instantaneous efficiency analysis shows that the magnetic tube has a higher top instantaneous efficiency as well as a higher heat loss coefficient, thus resulting a lower thermal efficiency as time passes and temperature rises. The temperature when the efficiency for the coating tube equals to that for the magnetic tube is about 53.8 °C and the temperature when the coating tube and the magnetic tube reach the same is about 73 °C. A comparison between the experimental results and what was available in literatures on the application of nanofluids to solar energy and a similar performance was observed.

17/02118 Heterogeneity in the adoption of photovoltaic systems in Flanders

De Groote, O. *et al. Energy Economics*, 2016, 59, 45–57.
The study considers the determinants of photovoltaic (PV) adoption in the Belgian region of Flanders, where PV adoption reached high levels during 2006–2012, because of active government intervention. Based on a unique dataset at a very detailed spatial level, the authors estimate a Poisson model to explain the heterogeneity in adoption rates. The following findings were obtained. First, local policies have a robust and significant impact on PV adoption. Second, there is a strong unconditional income effect, implying a Matthew effect in the subsidization of PVs. The third finding is however that this income effect is largely driven by the fact that wealthier households are more likely to adopt because they tend to be higher users, are more frequent house owners, or own houses that are better suited for PV. In several extensions, the authors consider the determinants of the average size of installed PVs, and the differential impact of certain variables over time.

17/02119 Highly reproducible and photocurrent hysteresis-less planar perovskite solar cells with a modified solvent annealing method

Zhou, Z. *et al. Solar Energy*, 2016, 136, 210–216.
Highly reproducible and photocurrent hysteresis-less inverted planar perovskite solar cells were demonstrated by a modified solvent annealing method in a two-step solution deposition (modified method). PbI_2 film was annealing at 40 °C using the residue solvent after spin-coating, which facilitated the subsequent $CH_3NH_3PbI_3$ perovskite active layer with high photovoltaic properties. The resulting device present a power conversion efficiency of 12.12%, which increased 42.7% compared with that of the control device fabricated as literatures.

17/02120 Influence of cycle time and collector area on solar driven adsorption chillers

Jaiswal, A. K. *et al. Solar Energy*, 2016, 136, 450–459.
Dynamic performance of a single-stage, two-bed, silica gel + water adsorption chiller operating in Bangalore, India is studied. Driving thermal energy is provided directly by an evacuated tube solar collector field. System dynamics are evaluated in the absence of thermal storage, which causes intra-day fluctuations in heat source and evaporator temperatures, which in turn influence the system performance. These dynamics are demonstrated for representative days in the months of April (summer) and December (winter). The focus is on the effect of variation of the collector area and the adsorption cycle time on the system performance. The maximum temperature of heat transfer fluid (water) is limited to 95 °C. The cyclic and daily averages of solar coefficient of performance ($DACOP_{sol}$) and cooling capacity ($DACC$) are used as key performance indicators. One of the key aspects of this study is to show that both of them can be maximized by suitably choosing the collector area and cycle time. Further, it is demonstrated that the solar driven adsorption chiller described here is ideally suited for cascading with an air-cooled R-134a vapour compression refrigeration system (VCRS). The variable throughput obtained from the solar adsorption chiller can help in liquid sub-cooling and hence to cover the deficit in cooling capacity of the VCRS arising due to high ambient temperature.

17/02121 Innovation subsidies versus consumer subsidies: a real options analysis of solar energy

Torani, K. *et al. Energy Policy*, 2016, 92, 255–269.
Given the interest in the commercialization of affordable, clean energy technologies, this study examines the prospects of solar photovoltaics (PV). The authors consider the question of how to transition to a meaningful percentage of solar energy in a sustainable manner and which policies are most effective in accelerating adoption. This paper develops a stochastic dynamic model of the adoption of solar PV in the residential and commercial sector under two sources of uncertainty – the price of electricity and cost of solar. The analytic results suggest that a high rate of innovation may delay adoption of a new technology if the consumer has rational price expectations. The authors simulate the model across alternative rates technological change, electricity prices, subsidies and carbon taxes. It is shown that there will be a displacement of incumbent technologies and a widespread shift towards solar PV in under 30 years – and that this can occur without consumer incentives and carbon pricing. It is shown that these policies have a modest impact in accelerating adoption, and that they may not be an effective part of climate policy. Instead, results demonstrate that further technological change is the crucial determinant and main driver of adoption. Further, results indicate that subsidies and taxes become increasingly ineffective with higher rates of technological change.

17/02122 Integrated voltage regulation in distribution grids with photovoltaic distribution generation assisted by telecommunication infrastructure

Leite, L. *et al. Electric Power Systems Research*, 2016, 136, 110–124.
Massive penetration of distributed generation photovoltaic systems (DGPV) connected to the power distribution grid through electronic inverters can contribute, in an aggregate scenario, to the performance of several power system control functions, notably in voltage regulation along a distribution feeder. In this context, the supervision and control of these generating units through a standardized, flexible and capillary communication infrastructure becomes a key factor in enabling large-scale integration. Present voltage regulation methods adopted in distribution grids using DGPV units are based on the local interaction of each source with the power grid, without exploiting the potential benefits of a wide integration among them. This paper proposes the use of an optimization method for voltage regulation, focused on reactive power injection control, based on a communication architecture model that coordinates the interaction among the inverters of DGPV units. This architecture enables each distributed source to perform in accordance with its operational characteristics and location, while dynamically coordinated by a distributed generation management system. The proposed communication infrastructure is based on the connectivity and interoperability requirements established by the international standard IEC 61850 and the IEEE 2030 reference model. A sensitivity analysis regarding the performance of voltage regulation and communication infrastructure, based on a co-simulation of PSCAD and MatLab, shows the effectiveness of the proposed optimization method. This work analyses the impact of communication network delay and unavailability in voltage regulation process.

17/02123 Investigating the collector efficiency of silver nanofluids based direct absorption solar collectors

Chen, M. *et al. Applied Energy*, 2016, 181, 65–74.
A one-dimensional transient heat transfer analysis was carried out to analyse the effects of the nanoparticle (NP) volume fraction, collector height, irradiation time, solar flux, and NP material on the collector efficiency. The numerical results were compared with the experimental results obtained by silver nanofluids to validate the model, and good agreement was obtained. The numerical results show that the collector efficiency increases as the collector height and NP volume fraction increase and then reaches a maximum value. An optimum collector height (~10 mm) and particle concentration (~0.03%) achieving a collector efficiency of 90% of the maximum efficiency can be obtained under the conditions used in the simulation. However, the collector efficiency decreases as the irradiation time increases owing to the increased heat loss. A high solar flux is desirable to maintain a high efficiency over a wide temperature range, which is beneficial for subsequent energy utilization. The modelling results also show silver and gold nanofluids obtain higher photothermal conversion efficiencies than the titanium dioxide nanofluid because their absorption spectra are similar to the solar radiation spectrum.

17/02124 Investigation on the effect of thermal resistances on a highly concentrated photovoltaic-thermoelectric hybrid system

Zhang, J. and Xuan, Y. *Energy Conversion and Management*, 2016, 129, 1–10.

A thermal analysis of a highly concentrated photovoltaic–thermoelectric (PV-TE) hybrid system is carried out in this paper. Both the output power and the temperature distribution in the hybrid system are calculated by means of a three-dimensional numerical model. Three possible approaches for designing the highly concentrated PV-TE hybrid system are presented by analysing the thermal resistance of the whole system. First, the sensitivity analysis shows that the thermal resistance between the TE module and the environment has a more great effect on the output power than the thermal resistance between the PV and the TE. The influence of the natural convection and the radiation can be ignored for the highly concentrated PV-TE hybrid system. Second, it is necessary to sandwich a copper plate between the PV and the TE for decreasing the thermal resistance between the PV and the TE. The role of the copper plate is to improve the temperature uniformity. Third, decreasing the area of PV cells can improve the efficiency of the highly concentrated PV-TE hybrid system. It should be pointed out that decreasing the area of PV cells also increases the total thermal resistance, but the raise of the efficiency is caused by the reduction of the heat transfer rate of the system. Therefore, the principle of minimizing the total thermal resistance may not be suitable for optimizing the area of PV cells.

17/02125 Linear equivalent models at the maximum power point based on variable weather parameters for photovoltaic cell

Li, S. *Applied Energy*, 2016, 182, 94–104.

In order to sweep completely the obstacle to the whole linearization of photovoltaic (PV) system with non-linear PV cell, in this paper, the voltage-current characteristic of PV cell at the maximum power point is linearized and two linear equivalent models including Thevenin equivalent model and Norton equivalent model are proposed. On the basis of this work, the whole linearization of PV system is workable and reasonable, and then the conventional linear theories or laws can be used to study PV system conveniently. Meanwhile, in this work, the direct relationships between three linear model parameters and variable weather parameters were found, which ensures the strong adaptation of these proposed models to the varying weather conditions. Finally, some simulation experiments verify that these proposed models are feasible and available in practical application, illustrate that the characteristics of three linear model parameters are influenced by varying weather conditions and unaffected by varying load, and show that PV system using the proposed Thevenin equivalent model has the same maximum power point tacking (MPPT) stead-state performance and similar MPPT transient-state performance with the conventional four-parameter model under fast varying weather conditions.

17/02126 Maximum power point tracking of photovoltaic systems based on the sliding mode control of the module admittance

Montoya, D. G. *et al. Electric Power Systems Research*, 2016, 136, 125–134.

Photovoltaic (PV) grid-connected applications use an adaption stage to extract the maximum power from the PV module matching its optimal operating point with the load operation. This paper presents a sliding mode control based on the admittance of the PV module to follow a reference provided by an external maximum power point tracking algorithm, and at the same time, to mitigate the perturbations generated by the load. The sliding mode controller is mathematically analysed, and a design process is proposed to ensure the desired performance in all the operation range. Finally, simulations and experimental results are used to demonstrate the efficiency of the proposed solution in the presence of both changes in the irradiance level and load perturbations.

17/02127 Maximum-power-point tracking during outdoor ageing of solar cells

Berginc, M. *et al. Solar Energy*, 2016, 135, 471–478.

This paper describes how to select a passive load which would the most accurately follow the maximum-power-point (MPP) of small laboratory size solar cells installed outdoors in central Europe. Either resistor or diode type of passive load have been used as a low-cost alternative to active MPP trackers (designed especially for a long-term outdoor stability study of different types of small size laboratory solar cells). The dye-sensitized solar cells have been chosen as a representative case since they exhibit similar current–voltage (I–V) characteristics dependence at different light intensities (G) and cell temperatures (T_C) as other solar cell's technologies. The results showed that the most efficient tracking was achieved when the I–V characteristic of the optimal resistor or diode cross the MPP of the solar cell measured at $G = 73\,\mathrm{mW/cm^2}$ and $T_C = 25\,^{\circ}\mathrm{C}$. A significantly better tracking could be obtained when instead of a resistor an optimal diode is used; the optimal diode consumes 96.5% of the annual energy that would be potentially produced by the solar cell connected to ideal MPP tracker while the optimal resistor consumes only 83.5% of that energy.

17/02128 Modelling concentrated solar power (CSP) in the Brazilian energy system: a soft-linked model coupling approach

Soria, R. *et al. Energy*, 2016, 116, 265–280.

Brazil is looking for innovative alternatives to supply the country's increasing electricity demand and provide flexibility to cope with higher shares of variable renewable energy (VRE). Concentrated solar power (CSP) can help solving this double challenge. Three energy planning tools, namely MESSAGE-Brazil, TIMES-TiPs-B and REMIX-CEM-B, have been combined to analyse the opportunities that CSP plants offer to the power system and to the wider energy system of the country. This work shows that CSP can be a cost-effective option under stringent mitigation scenarios. CSP can provide firm energy and dispatchable capacity in the north-east region of Brazil, optimally complementing wind and PV generations. Moreover, CSP can offer additional flexibility to the Northeast power system of the country, especially during winter, when the hydrological period is dryer. Results show synergies between CSP and other power supply technologies with small cost differences between the baseline and CSP-forced scenarios.

17/02129 Numerical and experimental investigation on a new type of compound parabolic concentrator solar collector

Zheng, W. *et al. Energy Conversion and Management*, 2016, 129, 11–22.

In order to improve the thermal efficiency, reduce the heat losses and achieve high freezing resistance of the solar device for space heating in cold regions, a new type of serpentine compound parabolic concentrator solar collector is presented in this paper, which is a combination of a compound parabolic concentrator solar collector and a flat plate solar collector. A detailed mathematical model for the new collector based on the analysis of heat transfer is developed and then solved by the software tool Matlab. The numerical results are compared with the experimental data and the maximum deviation is 8.07%, which shows a good agreement with each other. The experimental results show that the thermal efficiency of the collector can be as high as 60.5%. The model is used to predict the thermal performance of the new collector. The effects of structure and operating parameters on the thermal performance are mathematically discussed. The numerical and experimental results show that the new collector is more suitable to provide low temperature hot water for space heating in cold regions and the mathematical model will be much helpful in the designing and optimizing of the solar collectors.

17/02130 On recent advances in PV output power forecast

Raza, M. Q. *et al. Solar Energy*, 2016, 136, 125–144.

In last decade, the higher penetration of renewable energy resources (RES) in energy market was encouraged by implementing the energy polices in several developed and developing countries due to increasing environmental concerns. Among wide range of RES, photovoltaic (PV) electricity generation get higher attention by researcher, energy policy makers and power production companies due to its economic and environmental benefits. Therefore, a large PV penetration was observed in energy market with rapid growth in the last decade. The PV output power is highly uncertain due to several meteorological factors such as temperature, wind speed, cloud cover, atmospheric aerosol levels and humidity level. The inherent variability of PV output power creates different issues directly or indirectly for power grid such as power system control and reliability, reserves cost, dispatchable and ancillary generation, grid integration and power planning. Therefore, there is need to accurately forecast the PV output over the spectrum of forecast horizon at different chronological scales. In this paper, a comprehensive and systematic review of PV output power forecast models were provided. This review covers the different factors affecting PV forecast, PV output power profile and performance matrices to evaluate the forecast model. The critical analysis regressive and artificial intelligence based forecast models are also presented. In addition, the potential benefits of hybrid techniques for PV forecast models are also thoroughly discussed.

17/02131 Open-circuit switch fault tolerant wind energy conversion system based on six/five-leg reconfigurable converter

Shahbazi, M. *et al. Electric Power Systems Research*, 2016, 137, 104–112.

In this paper, a field programmable gate array-controlled fault tolerant back-to-back converter for doubly-fed induction generator-based wind energy conversion application is studied. Before an open-circuit failure in one of the semiconductors, the fault tolerant converter operates as a conventional back-to-back six-leg one. After the fault occurrence in one of the switches, the converter will continue its operation with the remaining five healthy legs. Design, implementation, simulation and experimental verification of a reconfigurable control strategy for the fault tolerant six/five-leg converter used in wind energy conversion are discussed. The proposed reconfigurable control strategy allows the

uninterrupted operation of the converter with minimum affection from an open-circuit switch failure in one of the semiconductors. Software reconfiguration is also necessary in pulse-width modulation signal generation unit, to assure that proper gate signals are calculated and generated based on the actual five-leg structure Simulations and experimental tests are carried out and the results are presented and compared. They all confirm the capability of the studied reconfigurable control and proposed fault tolerant architecture in ensuring the system's service continuity.

17/02132 Optimum band gap combinations to make best use of new photovoltaic materials

Bremner, S. P. *et al. Solar Energy*, 2016, 135, 750–757.

The detailed balance approach has been used to analyse the optimum use of band gaps in a multi-junction device of up to six sub-cells. Results for the AM1.5G spectrum suggest that as the number of sub-cells increases the importance of the bottom sub-cell band gap becomes less critical, assuming the optimum band gap combination for that value can be obtained. Given this greater freedom in choice, the potential for the use of silicon as an active substrate is investigated along with a cell thinning 'current sharing' approach to improve current mismatch in the device. Results show a more robust design space of multi-junctions with active silicon substrates when the current sharing approach is used, with performances close to the optimum for a completely free choice of band gaps. The use of the AM1.5D spectrum for a concentration ratio of 100, shows similar results for the substrate and a slight increase in band gap sensitivity for the upper band gaps in the stack. Inclusion of optical coupling between the sub-cells lowers limiting efficiency, with luminescent coupling mitigating the band gap sensitivity. The results and approach outlined are useful for determining how best to deploy new photovoltaic materials in multi-junction solar cells.

17/02133 Passive small scale electric power generation using thermoelectric cells in solar pond

Ding, L. C. *et al. Energy*, 2016, 117, 149–165.

Solar ponds have been widely utilized in providing low grade heat needed for industrial processes and for heating applications $<100\,^{\circ}C$. In this paper, a small scale passive electric power generation unit was devised for generating electricity from the heat available in the solar pond. The power generation unit proposed operates without the use of a pump and involves no moving parts. The design of the power generation unit was finalized after performing a comprehensive theoretical study on the possible geometrical arrangements. The power generation unit was fabricated and tested experimentally. The power generation unit consists of 120 commercially available thermoelectric cells accommodated in the outer and inner layers of this dual layer power generation unit. The power generation unit had produced a maximum power of 40.8 W under the condition of $T_h = 99\,^{\circ}C$. Under the normal operation of solar pond, the lower convective zone will have a temperature that lies within in the range of 40–80 °C. Thus, maximum output in the range of 19.5–27.4 W is more realistic for the system proposed with the heat to electric conversion efficiency ranges between 0.37% and 0.68%.

17/02134 Performance evaluation of a stand-alone solar dish Stirling system for power generation suitable for off-grid rural electrification

Kadri, Y. and Abdallah, H. H. *Energy Conversion and Management*, 2016, 129, 140–156.

The development of green power generation such as solar systems that have become a great interest for several countries especially for Tunisia as it presents a significant solar potential. For this purpose, this research has investigated the feasibility and the performance of standalone solar dish/Stirling micro generation plant for rural electrification. The considered hybrid system includes solar dish/Stirling engine, permanent magnet synchronous generator and a storage battery. To start with, thermal modelling and simulation have been carried out using Matlab for the solar-driven Stirling heat engine system composed of an Alpha Stirling engine, a solar collector and a receiver, in which the radiation, convection, conduction and radiation heat loss have been taken into consideration for the selected design. For numerical validation of the receiver's thermal model, simulation results were compared with experimental measurements reported for the EURODISH system with a reasonable degree of agreement. Second, the generated torque driving the generator has been estimated by the Adiabatic model of URIELI based on the classical fourth-order Runge–Kutta. In order for an autonomous control, the dish generator is connected to the load via power electronic converters where the bidirectional power flow is possible by the use of two voltage source converters in a back-to-back configuration. They are referred to as Stirling/generator side converter and load side inverter, both are oriented control by space vector pulse width modulation. In this context, the Stirling side converter is used to adjust the synchronous generator while the inverter controls the power flow between the direct current bus and the alternative side. Detailed tests of the proposed hybrid configuration was implemented in Matlab/Simulink software, by taking as a case study a measured load profile for a rural house and solar radiation data at the target area. The analysis of simulation results has shown that solar dish Stirling/synchronous generator system achieves the objectives of system autonomy and power supply stability. The effectiveness of the management strategy was also proved. It has been obtained that the variable speed Stirling/generator system is capable to feed an uncontrollable load under variations of climatic conditions during hot, moderate and cold seasons, in remote areas in Tunisia.

17/02135 Potential of rooftop solar photovoltaics in the energy system evolution of the United Arab Emirates

Griffiths, S. and Mills, R. *Energy Strategy Reviews*, 2016, 9, 1–7.

Solar power, and in particular solar photovoltaics (PV), is a rapidly growing source of energy in many regions of the world. However, the contribution of solar power in Middle East and North Africa (MENA) countries has been minor even though these countries possess some of the best levels of solar insolation globally. Recently, though, this has been changing. Changing hydrocarbon markets in the region, technology advances in solar PV and rapidly falling costs make solar power increasingly attractive to MENA countries that are actively diversifying their energy systems away from dependence on hydrocarbon fuel sources. Although utility-scale concentrating solar power and PV plants have been the focus through 2014, rooftop solar PV is being positioned to play potentially an important role in the United Arab Emirates (UAE)'s future energy mix. In this paper, rooftop solar PV in the UAE is taken as a case study for the evolution of a MENA energy system toward an increasingly sustainable power generation mix. The results show that rooftop solar PV can be an economically viable technology choice and hence will increasingly become part of regional energy strategies as technology costs continue to fall and tariff reforms continue to gain traction.

17/02136 Predictive energy management and control system for PV system connected to power electric grid with periodic load shedding

Syed, I. M. and Raahemifar, K. *Solar Energy*, 2016, 136, 278–287.

Power electric grid (PEG) tied photovoltaic (PV) plus battery energy storage stations (BESS) based microgrids (MG) are controlled and operated inefficiently with conventional energy management and control (CEMC) schemes. CEMC schemes, (1) leave these systems on the mercy of weather with either energy shortage resulting in loss of load (LOL) or requiring huge BESS resulting in high capital and operation & maintenance costs, (2) cause curtailment and thus wastage of surplus PV energy (PVE) and (3) increase energy cost due to unnecessary charging of BESS from PEG. LOL and surplus PVE wastage grow even further when MG are connected to a weak PEG with periodic load shedding. This paper proposes predictive energy management and control system (PEMCS) for PV + BESS MG tied to a weak PEG with periodic load shedding. Twenty-four hours of forecasts of load demand and PV potential with PEG load shedding schedule and BESS status are used as decision variables. The proposed PEMCS reduces PV energy (PVE) wastage due to curtailment, increases PV proportion locally and into PEG for PEG support, decreases unnecessary charging from the PEG, and increases savings for owner-consumer. The proposed scheme is simple, effective, and realistic, and accounts for errors in the forecasts. Results show increased proportions of PVE for both consumers and PEG, energy cost saving for consumers, and enhances weak PEG operational reliability.

17/02137 PVT type of the two-phase loop mini tube thermosyphon solar water heater

Ziapour, B. M. and Khalili, M. B. *Energy Conversion and Management*, 2016, 129, 54–61.

In this paper, the performance study is performed in order to verify the new design of the photovoltaic (PV) panel combined with type of the wickless heat pipe solar water heater. In this enhanced design, each wickless heat pipe is assumed in the shape of the loop mini tube comprised of the flow boiling process inside it. Without considering the PV panel, this design was reported in a prior published work by the authors. Here, the performance of the proposed passive PV–thermal (PVT) solar collector is numerically performed using EES software. The solar cell packing factor (i.e. fraction of the absorber plate area which is covered by the solar cells) is important parameter for designing a PVT system. The simulation results show that the thermal efficiency of the passive PVT solar system increases with increase of the solar cells packing factor. Through the simulation results it is found that the optimal numbers of the wickless heat pipes may be five loops. By selecting the five loops, the maximum value of the tank water temperature is obtained near to 72 °C in the evening. Also the maximum values of η_{th} and η_{pv} are found as 70% and 80% at noon time, respectively.

17/02138 Review of photovoltaic power forecasting

Antonanzas, J. *et al. Solar Energy*, 2016, 136, 78–111.

Variability of solar resource poses difficulties in grid management as solar penetration rates rise continuously. Thus, the task of solar power forecasting becomes crucial to ensure grid stability and to enable an optimal unit commitment and economical dispatch. Several forecast horizons can be identified, spanning from a few seconds to days or weeks ahead, as well as spatial horizons, from single site to regional forecasts. New techniques and approaches arise worldwide each year to improve accuracy of models with the ultimate goal of reducing uncertainty in the predictions. This paper appears with the aim of compiling a large part of the knowledge about solar power forecasting, focusing on the latest advancements and future trends. Firstly, the motivation to achieve an accurate forecast is presented with the analysis of the economic implications it may have. It is followed by a summary of the main techniques used to issue the predictions. Then, the benefits of point/regional forecasts and deterministic/probabilistic forecasts are discussed. It has been observed that most recent papers highlight the importance of probabilistic predictions and they incorporate an economic assessment of the impact of the accuracy of the forecasts on the grid. Later on, a classification of authors according to forecast horizons and origin of inputs is presented, which represents the most up-to-date compilation of solar power forecasting studies. Finally, all the different metrics used by the researchers have been collected and some remarks for enabling a fair comparison among studies have been stated.

17/02139 Solar dish concentrator for desalting water

Prado, G. O. *et al. Solar Energy*, 2016, 136, 659–667.

The purpose of this study was to build, characterize and analyse the performance of a solar dish concentrator for desalinating water. To build this device, an equatorial mount was adapted to track the sun, a satellite dish was mirrored and the distillation system was assembled using a glass flask, a copper tube and a silicone tube. The system was characterized experimentally based on the main parameters that define a solar concentrator. However, to determine the potential energy of the device, dynamic heating was simulated by computer and validated experimentally. Finally, to analyse the performance of the solar dish concentrator in terms of water desalination, experiments were conducted with semi-continuous insertion of saline solution containing concentrations of 0–4% of sea salt. The yield of distilled water varied of 4.95 kg/m^2 day (0%) to 4.11 kg/m^2 day (4%), a consequence of colligative effects. Therefore, a solar dish concentrator was built with a simplified distillation system whose yield per square metre provided sufficient drinking water to meet the daily needs of at least two adults.

17/02140 Solar flux density calculation for a heliostat with an elliptical Gaussian distribution source

Huang, W. and Sun, L. *Applied Energy*, 2016, 182, 434–441.

The calculation of solar flux density is a key work for the design and optimization of solar tower systems. Because of the amount of calculation, the source distribution is often regarded as a radial distribution, which is not consistent with the reality. This paper presents a new method to calculate the flux density distribution by a focusing heliostat with an elliptical Gaussian distribution source. The two-dimensional convolution integration is proposed and converted into a one-dimensional integration. The authors use the Gauss–Legendre integration method to reduce the amount of calculation and accelerate the speed of integration. This method can be used to calculate the solar flux at image and receiver plane by most of the heliostat. It needs only 0.1% time of the ray tracing method for calculating the efficiency of the heliostat. It can be applied for design optimization of the solar heliostat field which is superior to the present methods in both accuracy and computation requirements.

17/02141 Solar policy and practice in Germany: how do residential households with solar panels use electricity?

Wittenberg, I. and Matthies, E. *Energy Research & Social Science*, 2016, 21, 199–211.

A substantial amount of the over 1.5 million photovoltaic (PV) systems in Germany are installed in residential households. Among these households, those with the option of self-consumption, i.e. to consume self-generated electricity can reduce their electricity consumption, especially grid electricity, by load shifting and acting in an energy-efficient manner. The authors examined how electricity consumption is influenced by contextual and attitudinal factors. They administered an online questionnaire to 425 households with PV recruited from 15 PV-related web portals. The results showed that their electricity consumption was not lower than in other households, but environmental motivation was higher. Sufficiency attitudes and environmental motivation were predictors of engaging in energy-saving behaviours which in turn contributed to consumption reduction. Battery storage and automatic load shifting increased self-consumption. Evidence was found for a distinction between households with PV installation before and after grid parity was achieved, especially concerning moderation effects of the economic framework. To reduce electricity consumption, a combination of efficient technologies and more environmentally motivated energy-saving behaviours should be supported.

17/02142 Sub-100 °C solution processed amorphous titania nanowire thin films for high-performance perovskite solar cells

Wu, W.-Q. *et al. Journal of Power Sources*, 2016, 329, 17–22.

The present work demonstrates a facile one-step process to fabricate thin films of amorphous titania nanowires on transparent conducting oxide substrates via hydrolysis of potassium titanium oxide oxalate in an aqueous solution at 90 °C. The resultant titania nanowire thin films (that have not undergone further annealing) are efficient electron transport layers in $CH_3NH_3PbI_3$ perovskite solar cells, yielding full sun solar-to-electricity conversion efficiencies of up to 14.67% and a stabilized efficiency of 14.00% under AM 1.5G one-sun illumination, comparable to high temperature sintered TiO_2 counterparts. The high photovoltaic performance is attributed to the porous nanowire network that facilitates perovskite infiltration, its unique 1D geometry and excellent surface coverage for efficient electron transport, as well as suppressed charge recombination between fluorine-doped tin oxide and perovskite.

17/02143 The effect of current and prospective policies on photovoltaic system economics: an application to the US Midwest

Sesmero, J. *et al. Energy Policy*, 2016, 93, 80–95.

This study models fundamental features of current and prospective policies encouraging adoption of residential photovoltaic (PV) systems. A key finding is that time-of-day (ToD) pricing can enhance or worsen the economics of PV systems. Moreover, increased responsiveness of electricity demand to its price diminishes the effectiveness of ToD pricing in the absence of net metering, but does not affect it otherwise. An application to plausible conditions in the State of Indiana, USA, shows that current policies are unlikely to trigger adoption by a risk-neutral forward-looking residential customer. However, adoption of PV systems can be induced if the Federal Tax Credit is increased to cover 48% of capital cost (instead of the current 30%), which could imply a cost to the Federal Government of about $0.95/kW of installed capacity depending on the panel's size. The authors demonstrate that implementation of ToD pricing can trigger adoption under a range of on- and off-peak price combinations. But this analysis also shows that the cost-effectiveness of ToD pricing is enhanced at higher ratios of on-peak to off-peak prices.

17/02144 Thermal analysis of a heat pipe solar central receiver for concentrated solar power tower

Liao, Z. and Faghri, A. *Applied Thermal Engineering*, 2016, 102, 952–960.

A novel heat pipe solar central receiver for a molten salt solar power tower is presented. The basic element consists of a reflector, heat pipe, and receiver tube. The reflector redirects concentrated sunlight from the heliostats field onto the evaporator section of the heat pipe. After absorbing the radiative heat energy, the working fluid inside the heat pipe is vaporized at the evaporator section, and flows to the condenser section of the heat pipe where it condenses. The condenser section is inserted into the receiver tube, and is cooled by a cross flow of the heat transfer fluid inside the receiver tube. In the proposed concept, the receiver tube is free from direct irradiation by the sunlight and therefore can be kept warm by electrical heating. This will extend the daily operating time of the receiver and greatly reduce possible freezing of the molten salt. In this study, a cavity receiver with the same geometry and boundary conditions as the molten salt electrical experiment (MSEE) cavity receiver was developed. Numerical simulation for the basic element of the cavity receiver was conducted. An 88.5% efficiency was obtained, which is slightly higher than the MSEE. Moreover, the receiver efficiency under a different number of flow passes and various heat flux density on the absorbing surface was also studied. Results show that the receiver efficiency can be as high as 91.5%.

Wind energy

17/02145 Coordinated planning of large-scale wind farm integration system and regional transmission network considering static voltage stability constraints

Gan, L. *et al. Electric Power Systems Research*, 2016, 136, 298–308.

The incoordination between centralized wind power development and transmission planning is the main cause of wind power curtailment. Moreover, engineering practice shows that voltage issue may trigger large-scale tripping-offline contingency of wind turbines. With the

objective of optimum economy, a coordinated planning method of large-scale wind farm integration system and relevant regional transmission network was proposed considering static voltage stability in this paper. A practical criterion of static voltage stability was formulated as operational constraints in the proposed model to ensure the obtained scheme to be technically and economically optimal. Raster map and disjunctive inequalities were introduced to linearize the model such that the model can be solved by mixed integer linear programming solvers directly. Numerical simulations show the validity and rationality of the proposed coordinated planning method.

17/02146 Deciding on the support schemes for upcoming wind farms in competitive electricity markets

Zamani-Dehkordi, P. *et al. Energy*, 2016, 116, 8–19.

A variety of policies have driven escalated global growth of wind power generation in recent years. However, wind production should be supported through market-based schemes that avoid overcompensation. The present paper aims to determine a justified support scheme for upcoming wind farms in competitive electricity markets. Clustering tools and non-parametric regression algorithms are employed to model the price-formation process in the market and estimate the revenue of forthcoming wind facilities. Accordingly, the premium paid to an upcoming wind farm is calculated by incorporating its estimated revenue and levelized cost of energy. Then, the impact of the proposed wind project on wholesale and retail electricity prices is modelled based on the achieved non-parametric regression models. The methodology is applied to two wind farms in the Alberta and Ontario electricity markets in Canada as the case studies. The results indicate that electricity consumers in Ontario should pay a higher premium for each unit of energy generated by the wind farm due to its lower revenue from the market. However, it is observed in both markets that the impact of wind farms on wholesale prices exceed the remuneration paid to them and thus, electricity consumers experience a decrease in their ultimate electricity costs.

17/02147 Double input Z-source inverter applicable in dual-star PMSG based wind turbine

Dehghanzadeh, A. R. *et al. International Journal of Electrical Power & Energy Systems*, 2016, 82, 49–57.

This paper proposes a new double-input Z-network for application in wind energy conversion system (WECS) which is composed of two same DC voltage sources as input sources, two inductors and one capacitor. As a result, the presented structure requires less capacitor number compared to traditional Z-network and it will be able to deliverer energy of both DC sources to local load or grid. The proposed inverter is applicable in dual-star PMSG based WECS, since it requires two DC voltage sources in same value. Besides, dynamic modelling of dual-star PMSG is presented to analyse proposed WECS connected to grid which employs dual-star PMSG and double-input Z-source inverter. The proposed dual-input Z-source inverter controls maximum power point tracking (MPPT) and delivering power to the grid. Therefore, other DC–DC chopper is not required to control two sets of rectified output voltage of generator in view of MPPT. As a result, the proposed topology requires less power electronic switches and the suggested system is more reliable against short circuit. The ability of proposed WECS with dual-star PMSG and double-input Z-source inverter is validated with simulation results and experimental tests using PCI-1716 data acquisition system.

17/02148 Fault diagnosis and condition monitoring of axial-flux permanent magnet wind generators

Ogidi, O. O. *et al. Electric Power Systems Research*, 2016, 136, 1–7.

This paper presents fault detection techniques in an attempt to discriminate between two common faults in axial-flux permanent magnet wind generators namely; static eccentricities and interturn short circuit faults. A combination of condition monitoring systems is proposed to achieve the discrimination; with detection techniques derived from current and vibration signatures for both faults using signal processing techniques. Parametric spectral estimation technique is applied as an alternative to the Fourier transform to process the fault signatures. This effectively overcame the problem of non-stationarity of signals due to variable wind speed as high frequency resolution was attained with less than three seconds of measurement data. The results will advance the development of standards and technical guidelines in the condition monitoring of permanent magnet synchronous generators in wind turbines.

17/02149 Marine wind energy and the North Sea offshore grid initiative: a multi-level perspective on a stalled technology transition?

Flynn, B. *Energy Research & Social Science*, 2016, 22, 36–51.

Building electricity grids at sea implies a radical transformation of grid topologies. In time, a marine super-grid is conceivable. If growing numbers of subsea electricity cables are meshed with marine renewable, a 'greening' of such grids is also possible. Based on interview research, this paper examines one such ambitious proposal: the Northern Seas Countries Offshore Grid Initiative (NSCOGI). The multi-level perspective (MLP) on technology transitions is used to evaluate progress to date. Obstacles uncovered include competing and still immature grid technology niches. There is only equivocal support from key actors within the relevant socio-technical electricity regime. National grid transmission system operators appear more interested in subsea cables to trade electricity rather than enhancing marine renewables. While the EU might be assumed to be a vital actor to support a North Sea grid, it has only limited influence. National policy insiders and decisions matter more. This paper stresses the residual importance of the national level for offshore wind and electricity grids. A marine super-grid wired up with offshore wind-farms throughout the North Sea, is both more tentative in its emergence, but also ambiguous in its support for offshore wind.

17/02150 Multi-parameter bifurcation analysis of subsynchronous interactions in DFIG-based wind farms

Revel, G. *et al. Electric Power Systems Research*, 2016, 140, 643–652.

This work analyses the dynamics involved in subsynchronous interactions between wind farms and series-compensated transmission lines. This adverse phenomenon may arise when doubly-fed induction generators are radially connected to an AC transmission line with series capacitive compensation. The resulting subsynchronous oscillations can produce the system instability and cause a severe damage to the wind turbines. The study is carried out combining tools from bifurcation theory, eigenvalue analysis and non-linear time-domain simulations. The impact on the subsynchronous mode due to the variation of a set of key parameters is considered. These parameters include the series compensation of the transmission line, the wind speed (generated power), the wind energy penetration level, and a gain of the internal control loop of the wind turbine. The bifurcation study determines that the underlying mechanism associated with the appearance of subsynchronous oscillations can be explained by means of Hopf bifurcations of the equilibrium point and their corresponding limit cycles. In addition, the saturation of the wind turbine converters plays an important role in the dynamics, introducing non-smooth bifurcations that are also analysed.

17/02151 Numerical and experimental comparison between two different blade configurations of a wind generator

Alaimo, A. *et al. Composite Structures*, 2016, 136, 526–537.

This paper presents a comparison between the structural behaviour of a wind generator with straight blades and a composite prototype of a wind generator with helical blades. Numerical structural analyses are performed by means of finite element models by using the ANSYS Mechanical software package. Furthermore, laboratory dynamic experimental tests are carried out on real-scale specimens of the two wind generator configurations in order to find their modal properties in terms of natural frequencies and modal shapes. The results of the experimental campaign are then used to update the numerical models by minimizing an objective function. Total stresses and deformations of the two wind generator configurations, coming from the updated numerical models, are evaluated and compared to quantitatively point out the improvement of the structural behaviour obtained by the use of composite materials.

17/02152 Participation of PMSG-based wind farms to the grid ancillary services

Abbes, M. and Allagui, M. *Electric Power Systems Research*, 2016, 136, 201–211.

With the increased penetration of wind energy in many utility grids throughout the world, transmission system operators (TSO) are facing further difficulties regarding power system control and stability. Therefore, modern wind farms should participate to the primary voltage and frequency control of power systems. This paper presents the design of a supervisory control strategy for grid-connected wind farms. Wind turbines within the investigated wind farm are pitch controlled and use the direct drive technology. It has a total installed capacity of 50 MW and it includes 25 permanent magnet synchronous generator (PMSG)-based wind turbines with a rated power of 2 MW each. The proposed supervisor is developed with all features that make the wind farm able to provide active and reactive power control. It includes automatic voltage and frequency control with droop and dead band. Performances of this supervisor are evaluated in terms of compliance with the Danish TSO requirements.

17/02153 Simulating the wake flow effect of wind turbines on velocity and turbulence using particle random walk method

Song, M. X. *et al. Energy*, 2016, 116, 583–591.

This paper presents a novel way of simulating the effect of velocity decay and turbulence of wind turbine's wake flow. By decoupling the solving of wake flow from that of the velocity field, the proposed model treats the wake flow intensity as a kind of convective and diffusive

virtual matter. The particle random walk method is utilized to simulate the motion of the virtual matter. Comparing to the existing linear model for turbine wake flow, the proposed model can predict the distributions of velocity decay and turbulence of wake flow in a non-uniform flow field above complex terrain. Experimental data from wind tunnel and real wind farm is used to validate the model, demonstrating its effectiveness on estimating the velocity decay and the turbulence intensity, and additionally, the power yield of a wind farm. The model proposed in this paper can be integrated into algorithms for numerical assessment and micro-siting optimization of wind farms on complex terrains.

17/02154 Static test until structural collapse after fatigue testing of a full-scale wind turbine blade
Lee, H. G. and Park, J. *Composite Structures*, 2016, 136, 251–257.
The effect of fatigue damage on the residual strength of a large wind turbine blade is a very important issue in the wind power industry. To test the residual strength after fatigue testing, this study prepared a test specimen, a 48.3 m wind turbine blade that had experienced initial static tests and then fatigue tests in accordance with the technical specification IEC TS 61400-23. The prepared specimen was loaded sequentially along the positive flapwise, the positive edgewise, and the negative flapwise direction, while video-recording the test situations. The wind turbine blade was able to sustain the loads in the first two tests, but the blade collapsed in the third test when the negative flapwise load reached 70% of the maximum target value, a value representing 50% of the most severe load in the first test. Based on the recorded information and the fracture patterns at the blade's broken section, the collapse processes were analysed. From this analysis a modified laminate pattern is suggested that can enhance the residual strength of a fatigue damaged wind turbine blade.

17/02155 Towards realistic design of wind dams: an innovative approach to enhance wind potential
Tajeddin, A. and Fazelpour, F. *Applied Energy*, 2016, 182, 282–298.
In an attempt to discover alternative energy sources to fossil fuels, renewable energy sources (RES) have gained considerable attention in recent years. RESs are also represented as clean sources; producing comparatively lower greenhouse gas emissions. Among RESs, wind energy is one of the most abundant and increasingly cost-competitive energy resources, and it is becoming the fastest growing source of electricity in the world. Regarding the improvement of wind power, one of the key aspects that must be considered is achieving enhanced reliability and efficiency at once. This study introduces and applies an innovative method to make a wind dam, which is a new approach to wind farms' site selection for production of electricity. The proposed method enhances the wind potential by means of a natural or artificial barrier such as a hill, and is supported by analytical expressions and computational fluid dynamics (CFD) models. A systematic case study has been designed at a site near the city of Tehran, Iran, and an analytical method has been applied that includes meteorological data analysis, CFD modelling along with energy power and economic assessment.

17/02156 Trading wind power with barrier option
Xiao, Y. *et al. Applied Energy*, 2016, 182, 232–242.
The emerging renewable power system entails competition-driven instead of non-competitive regulations for wind power. An increasing amount of wind power is therefore traded in pool market. Due to wind power's fluctuation and randomness, wind power producers (WPPs) suffer from risks of both power generation and market price. Based on the proposed WP-traded (wind power-traded) price and equivalent WPP-traded quantity, this work devises a barrier option for wind power, with which WPPs can trade their hedged proportion of power at prices no less than a predetermined strike price during the option life. The optimal purchasing framework and negotiation process are provided both in pool market and with bilateral contract. Case studies based on the Iberian market are conducted to verify the applicability of the proposed barrier option. The results show notable benefits of the barrier option in improving WPP's utility. The bilateral contract takes advantage of customer's elastic demand to countervail WPP's power deviations and charges customer a lower price. Furthermore, Efficiencies of barrier option and bilateral contract are mutually promoted as barrier option results in lower price and larger boundary range of bilateral contract, while bilateral contract leads to less possibility on over-hedging and better utilization of barrier option.

17/02157 Transmission expansion planning in the presence of wind farms with a mixed AC and DC power flow model using an imperialist competitive algorithm
Moradi, M. *et al. Electric Power Systems Research*, 2016, 140, 493–506.
Renewable generation and distributed resources are becoming increasingly relevant due to their various advantages and intense regulatory support. Therefore, there is a need to consider the effects of these new sources in the transmission network. In addition, the accurate assessment of losses is necessary in order to evaluate the impact of distributed generation. This paper presents a single-objective optimization method that is applied to different case studies that include an AC and a DC power flow in order to consider losses accurate and efficiently. The proposed algorithm considers uncertainty in wind generation and demand, as well as the costs for investment, repair, maintenance, and losses. This problem is solved using an imperialist competitive algorithm (ICA), a meta-heuristic method that has been proposed recently and has shown promising results compared to the other well-established evolutionary methods such as genetic algorithm (GA). The proposed method is investigated on the IEEE 24-bus and IEEE 118-bus test systems. The results are compared to the results reported in the literature. The results confirm that an accurate evaluation of losses using an ACPF does modify the optimal plan and hence it is important to include an ACPF when performing transmission expansion planning. In addition, the implemented ICA displays a more efficient performance than a plan GA in the same case study.

Others, including economics

17/02158 A high-resolution assessment of wind and wave energy potentials in the Red Sea
Langodan, S. *et al. Applied Energy*, 2016, 181, 244–255.
This study presents an assessment of the potential for harvesting wind and wave energy from the Red Sea based on an 18-year high-resolution regional atmospheric reanalysis recently generated using the advanced weather research forecasting model. This model was initialized with ERA-Interim global data and the Red Sea reanalysis was generated using a cyclic three-dimensional variational approach assimilating available data in the region. The wave hindcast was generated using WAVEWATCH III on a 5-km resolution grid, forced by the Red Sea reanalysis surface winds. The wind and wave products were validated against data from buoys, scatterometers and altimeters. This analysis suggests that the distribution of wind and wave energy in the Red Sea is inhomogeneous and is concentrated in specific areas, characterized by various meteorological conditions including weather fronts, mesoscale vortices, land and sea breezes and mountain jets. A detailed analysis of wind and wave energy variation was performed at three hotspots representing the northern, central and southern parts of the Red Sea. Although there are potential sites for harvesting wind energy from the Red Sea, there are no potential sites for harvesting wave energy because wave energy in the Red Sea is not strong enough for currently available wave energy converters. Wave energy should not be completely ignored, however, at least from the perspective of hybrid wind-wave projects.

17/02159 A method for the behavioral analysis of partial discharges in hydrogenerators by generalized linear models
Gomes, F. J. S. *et al. Electric Power Systems Research*, 2016, 140, 284–287.
This study proposes a method for the analysis of partial discharges in hydrogenerators through generalized linear models from data collected by capacitative couplers associated to phases A, B and V for the measurement of partial discharges in the stator windings of a hydrogenerator located at a hydroelectric plant. The dependent variable was considered the number of partial discharge events, explained by the variables of amplitude and phase angle. The applied models used to represent the data were the Poisson and negative binomial models. The latter showed the best fit. With the estimates of the model, it was possible to observe that the probability of partial discharge occurrence increased for low amplitude intervals and that these were distributed throughout all angle classes.

17/02160 A non-isolated three-phase high step-up DC–DC converter suitable for renewable energy systems
Nouri, T. *et al. Electric Power Systems Research*, 2016, 140, 209–224.
This paper proposes a non-isolated three-phase high step-up DC–DC converter based on three-winding high frequency coupled-inductor (HFCI) and voltage multiplier cell (VMC). The primary and secondary windings of each HFCI are inserted in the same phase and the tertiary winding is inserted in one of the two other phases. Combining the advantages of both HFCIs and VMCs, the voltage conversion ratio is increased and the voltage across the semiconductors is decreased. The converter analysis is given in three modes of operation named as continuous conduction mode, discontinuous conduction mode and boundary conduction mode. The experimental results are finally provided to show the validity of the proposed converter scheme.

17/02161 A real options model for renewable energy investment with application to solar photovoltaic power generation in China

Zhang, M. M. *et al. Energy Economics*, 2016, 59, 213–226.

This paper proposes a real options model for evaluating renewable energy investment by considering uncertain factors such as CO_2 price, non-renewable energy cost, investment cost and market price of electricity. A phase-out mechanism is built into the model to reflect the long-term changes of subsidy policy. The authors apply the proposed model to empirically evaluate the investment value and optimal timing for solar photovoltaic power generation in China. These empirical results show that the current investment environment in China may not be able to attract immediate investment, while the development of carbon market helps advance the optimal investment time. A sensitivity analysis is conducted to investigate the dynamics of investment value and optimal timing under the changes of unit generating capacity, subsidy level, market price of electricity, CO_2 price and investment cost. It is found that the high investment cost and the volatility of electricity and CO_2 prices, are not conducive to attract immediate investment. Instead, increasing the level of subsidy, promoting technological progress and maintaining the stability of market are useful to stimulate investment.

17/02162 An assessment of the economic and environmental feasibility of evaporative cooling unit

Jaber, S. *Applied Thermal Engineering*, 2016, 103, 564–571.

Performance of indirect evaporative air-conditioning (IEAC) is strongly influenced by the climate conditions and varies widely in different climate zones. This investigation conducts thermal and economic performance analysis of IEAC under climatic conditions of three cities from different zones: Amman, Aqaba and Berlin. Based on the hourly climate data of each zone, economic assessment of IEAC is estimated using life cycle cost and payback period criterion according to economic figures from local markets for each location. The results revealed that IEAC is promising technology in the selected climate zones. A well-optimized IEAC can cover 99.98%, 95.26% and 84.83% from annual cooling demand in Berlin, Amman and Aqaba, respectively.

17/02163 Assessing solution quality and computational performance in the hydro unit commitment problem considering different mathematical programming approaches

Finardi, E. C. *et al. Electric Power Systems Research*, 2016, 136, 212–222.

This paper presents a comparative analysis of different mathematical programming approaches for optimizing the hydro unit commitment (HUC) problem with cascaded plants, multiple generating units, and a head-dependent hydropower model. Regarding the HUC problem related to this paper, the objective is to minimize the cascade outflow while satisfying all constraints, including a power target for each plant, in a day-ahead planning horizon. The decision variables are the on/off status of the units and the respective generation levels. Rigorously, the HUC is a mixed-integer non-linear programming (MINLP) problem, and several strategies can be used to compute near-optimal solutions. In this paper, the authors are interested in accessing the solution quality, as well as the computational performance when the HUC problem is solved using the following mathematical programming approaches: (i) the Lagrangian relaxation that represents a decomposition technique that exploits the HUC modelling structure, (ii) a MINLP solver that can handle the size and the non-concavity of the problem, and (iii) a mixed-integer linear programming approach obtained by means of the hydropower model linearization. To perform the proposed analysis, numerical results are presented related to a real hydro system with eight cascaded reservoirs and 29 generating units.

17/02164 Can local government play a greater role for community renewable energy? A case study from Australia

Mey, F. *et al. Energy Research & Social Science*, 2016, 21, 33–43.

Despite unsupportive political conditions for renewable energy (RE) in Australia, a new movement is emerging. About 70 Australian community groups have started to embrace the concept of community renewable energy (CRE) and develop their own projects. However, faced with a complex institutional environment and the absence of national government support, only a few groups have established operating CRE projects as yet. In this situation the role of local government (LG) 'closest to the people' deserves more attention. By presenting empirical evidence from an Australia-wide survey and a number of semi-structured interviews, the authors identified motivations, barriers and opportunities of LGs in RE deployment, giving special attention to the role LGs in enabling CRE initiatives. This survey found that RE generation by LGs has become a widespread budget relevant activity. The majority of LGs have yet to recognize the social benefits associated with a community collaboration in the field of RE. However perceived financial and regulatory barriers limit the scope of action for LGs and their communities, and higher-level government support is essential. The Australian experience is relevant to other countries with similar political and institutional barriers.

17/02165 CVaR constrained planning of renewable generation with consideration of system inertial response, reserve services and demand participation

Inzunza, A. *et al. Energy Economics*, 2016, 59, 104–117.

Integration of renewable generation can lead to both diversification of energy sources (which can improve the overall economic performance of the power sector) and cost increase due to the need for further resources to provide flexibility and thus secure operation from unpredictable, variable and asynchronous generation. In this context, the authors propose a cost-risk model that can properly plan generation and determine efficient technology portfolios through balancing the benefits of energy source diversification and cost of security of supply through the provision of various generation frequency control and demand side services, including preservation of system inertia levels. The authors use a scenario-based cost minimization framework where the conditional value at risk (CVaR), associated with costs under extreme scenarios of fossil fuel prices combined with hydrological inflows, is constrained. The model can tackle problems with large data sets (e.g. 8760 hours and 1000 scenarios) since the authors use linear programming and propose a Benders-based method adapted to deal with CVaR constraints in the master problem. Through several analyses, including the Chilean main electricity system, this study demonstrates the effects of renewables on hedging both fossil fuel and hydrological risks; effects of security of supply on costs, risks and renewable investment; and the importance of demand side services in limiting risk exposure of generation portfolios through encouraging risk mitigating renewable generation investment.

17/02166 Demystification and localization in the adoption of micro-hydro technology: insights from India

Höffken, J. I. *Energy Research & Social Science*, 2016, 22, 172–182.

The phrase 'small is beautiful' holds true for the micro-hydro plants discussed in this article. Micro-hydro plants can convert the energy of falling water into electricity. In India, access to electricity cannot be taken for granted, especially in rural areas, which do not yet have grid extension or where it is too costly or infeasible. In these cases, micro-hydro plants are a welcome solution. Here the author discusses the efforts of two non-governmental organizations, a private company, and a government agency, to facilitate micro-hydro projects in India, thereby increasing the socio-economic empowerment of rural inhabitants without electricity access. Based on extensive ethnographic data and constructivist conceptualizations of scale and consequences it is found that these projects can indeed be described as 'beautiful' technology interventions. In line with the common discourse on 'small is beautiful', the projects emphasize community engagement, control and locality. Yet, importantly, they are 'beautiful' in diverse ways. The actors set different priorities when implementing their small-scale technology interventions. Highlighting these priorities is important because they can empower people to acquire different roles, ranging from engaged consumers to prosumers. Instead of solely concentrating on the (small) scale of a technology the significance of implementing these interventions should be considered.

17/02167 Development of the methodology for the evaluation of a hydro-pumped storage power plant: Swiss case study

Iliadis, N. A. and Gnansounou, E. *Energy Strategy Reviews*, 2016, 9, 8–17.

During the last two decades, an evolving market structure is recognized starting from the spot market and its derivatives, resulting to several other markets such as the intraday market (IM), the balancing market (BM) and the reserve capacity market (RCM). The participation in these markets has changed significantly the operation policy of the plants and, consequently, their value in the market. The current paper deals with the problem of the long-term valuation of a hydroelectric pump storage (HPS) plant participating in the DAM and IM. For this purpose, an appropriate methodology has been developed while it is demonstrated on a real case study concerning the operation of a Swiss based HPS plant that participates in the DAM and IM of the German electricity market, for a horizon of 35 years.

17/02168 Effect of mooring-line stiffness on the performance of a dual coaxial-cylinder wave-energy converter

Wang, L. *et al. Applied Ocean Research*, 2016, 59, 577–588.

A point-absorber-type wave-energy converter (WEC) consisting of a floating vertical inner cylinder and an annular outer cylinder that slides along the inner one is considered. The two cylinders heave differently under wave excitation, and wave energy can be harnessed from the relative heave motion between the two cylinders using a permanent magnet linear generator as the power take-off unit. A mooring cable is

attached to the bottom of the inner cylinder. This paper aims to examine the effect of the stiffness of the mooring cable on the performance of the coaxial-cylinder WEC system. The two limiting cases of no mooring cable (freely floating inner and outer cylinders) and an infinitely stiff mooring cable (fixed inner cylinder) were also considered. To perform the analysis, hydrodynamic and interference coefficients of the two heaving cylinders were computed semi-analytically using the method of matched eigenfunction expansions. Experimentally determined viscous corrections on damping were also included in the model in order to have more realistic predictions. The performance of the system in terms of motion responses and capture width were predicted and discussed for both regular and irregular waves. The results of the analysis indicate that both the freely floating design and the design with rigidly moored inner cylinder are viable. The two limiting cases show similar optimal performances, albeit with very different optimal generator damping. However, an ill-chosen mooring-cable stiffness may cause the inner and the outer cylinders to have the same resonance frequency, eliminating the relative heave motion and leading to almost no energy extraction. This situation needs to be avoided when designing the mooring system for a coaxial-cylinder WEC.

17/02169 Energy and reserve co-optimization within the short term hydrothermal scheduling under uncertainty: a proposed model and decomposition strategy

Salgado, C. J. L. *et al. Electric Power Systems Research*, 2016, 140, 539–551.

Procurement of spare capacity is an essential mechanism in electric power systems. Through it the system is able to endure the disturbances induced by different sources of uncertainty, which also impact the system's operational cost. This paper introduces an optimization model for the short-term hydrothermal scheduling that performs a co-optimization of energy and reserves for tertiary regulation, considering hydrology uncertainty and forced outages of generation units and transmission lines. The formulation presented is extended to consider intermittent stochastic generation from wind farms or hydro plants without storage capability. This work also proposes a decomposition scheme to deal with the resulting stochastic and large scale optimization problem. The proposed strategy relies on a coordinated application of two instances of the Bender's decomposition principle. By means of two study cases it will be demonstrated the effectiveness of the proposed model and the performance of the methodology.

17/02170 Financial development and deployment of renewable energy technologies

Kim, J. and Park, K. *Energy Economics*, 2016, 59, 238–250.

Using a unique panel data set of 30 countries for the 2000–2013 period, the authors examine whether financial market development promotes the deployment of renewable energy on a global scale. In particular, they conjecture that countries with well-developed financial markets experience growth in the renewable energy sector due to easier access to external financing. It was found that renewable sectors that are relatively more dependent on debt and equity financing grow disproportionately faster in countries with developed financial markets. These results support the view that financial development leads to a reduction in CO_2 emissions by addressing the role of financial markets in deploying renewable energy.

17/02171 Integration of storage and renewable energy into district heating systems: a review of modelling and optimization

Olsthoorn, D. *et al. Solar Energy*, 2016, 136, 49–64.

The building and infrastructure sector is accountable for 46% of the total worldwide energy consumption. Most traditional energy sources such as coal or petroleum are among the non-renewable types and most likely to be depleted in the forthcoming decades. To address the current energy crisis, use of renewable energy such as solar sources and a considerable increase in energy efficiency are proposed as the potential solutions. District heating systems (DHS), in particular, has recently received more attention due to several advantages in energy production, distribution and consumption for the space heating. This paper reviews the recent advancements in the energy production, modelling and optimization of the DHSs. A classification of energy sources is presented in terms of their sustainability and ease of integration to a DHS. Current modelling methods are further compared with respect to computational limitations, level of precision as well as the degree of certainty in the output level. Moreover, the recent studies of DHS are classified in accordance with the optimization objectives, including energy/exergy efficiency, cost, exergo-economic/thermo-economic and greenhouse gas and pollutant production.

17/02172 Numerical energy balance analysis for an onshore oscillating water column–wave energy converter

Elhanafi, A. *et al. Energy*, 2016, 116, 539–557.

The hydrodynamic performance of oscillating water column (OWC) wave energy converters depends mainly on the behaviour of the wave–OWC interaction. In this paper, a fully non-linear 2D RANS-based computational fluid dynamics (CFD) model was used to carry out an energy balance analysis of an onshore OWC. Chamber differential air pressure and free surface elevation from published physical measurements were used to validate the CFD model. Additional validation was carried out via PIV data from available model-scale experiments to validate the CFD model's capability in capturing the flow field and the turbulent kinetic energy. The validated CFD model was then used in an extensive campaign of numerical tests to quantify the relevance of different design parameters such as incoming wave height and turbine pneumatic damping to characterize the hydrodynamic performance and wave energy conversion chain of the OWC. To capture the flow field inside the OWC in good agreement, additional refinement was required at the field of view together with utilizing either SST or RSM turbulence models rather than k-ε. It is found that the applied damping has crucial impacts on the energy conversion process. Also, increasing the wave height can lead to a massive drop in the system efficiency. Furthermore, both power take-off damping and wave height play an important role in vortex formation around the upper and lower chamber's lips during the in-flow and out-flow stages.

17/02173 Optimal sizing of a wind-photovoltaic-battery hybrid renewable energy system considering socio-demographic factors

Tito, S. R. *et al. Solar Energy*, 2016, 136, 525–532.

The sizing of a stand-alone wind–photovoltaic-battery hybrid renewable energy system (HRES) is greatly influenced by socio-demographic factors however, few studies have examined how socio-demographic factors, as borne out by different electrical usage patterns, influence the size of HRESs. This paper investigates how these factors influence the optimal sizing of a stand-alone HRES using a hybrid optimization method to match the available renewable energy with the demand. In this regard, different energy usage patterns resulting from users' socio-demographic profile have been investigated and used for the optimal sizing of a HRES. The results show that the electricity usage profile of a site has a significant impact on the sizing and design of the system. Further, the results illustrate that one can design a system that meets the demand profiles resulting from socio-demographic factors with a minimum unmet load; however, by optimizing systems to the users socio-demographic profile, significant cost savings can be made.

17/02174 Promoting the surge immunity techniques of an uninterruptible hydro plant power system under the surge environment of high exposure

Chen, C.-R. *et al. International Journal of Electrical Power & Energy Systems*, 2016, 82, 274–280.

Uninterruptible power systems in hydro plants under the surge environment of high exposure are susceptible to surge impact. In order to solve the problems of equipment malfunctions or failures caused by the surge, this paper applies the principle of surge energy transfer to design a low-voltage surge protection circuit, which prevents the surge from interfering with or damaging UPS devices. According to the IEEE and IEC standards test requirements, after the actual loads are connected to the load side of this circuit, surge generators are used to test the surge immunity of the surge protection circuit and actual load; test results confirm that the surge protection circuit proposed in this paper is effective for the protection of surge interference at low-voltage.

17/02175 Semi-physical piecewise affine representation for governors in hydropower system generation

Donaisky, E. *et al. Electric Power Systems Research*, 2016, 136, 181–188.

This paper presents a non-linear model for a hydraulic amplifier, a component of the governor in the speed control loop of hydroelectric power plants. The amplifier transforms the electrical signal of the controller into mechanical movement of the turbine components, including the switching characteristics. This model is used to propose, on the one hand, a piecewise affine (PWA) representation for the hydraulic amplifier, and, on the other hand, a methodology for estimating the model parameters using field measurements, which facilitates its practical implementation. This representation is referred to as semi-physical because the model parameters are closely related with the physical construction of the hydraulic amplifier components. Among the advantages of this PWA representation are the appropriate structuring for use in system identification methods, for estimating its parameters, and the existence of advanced control techniques that use this structure in controller design, thereby improving the load-frequency control performance. The paper concludes with a description of the results, including the parameters that were estimated by using the hydraulic amplifier model with PWA structure.

17/02176 Sensitivity analysis in the technical potential assessment of onshore wind and ground solar photovoltaic power resources at regional scale

Bossavy, A. *et al. Applied Energy*, 2016, 182, 145–153.

Potential assessment has served various objectives in the development of renewable energies. However, the prospective nature of this type of assessment sometimes makes it difficult to evaluate and compare estimation results based on different data and modelling. To facilitate this comparison, uncertainty estimates need to be systematically provided. Since potential assessment sometimes relies on numerous parameters, this may first require determining the most important inputs to focus on. This paper proposes a sensitivity analysis methodology based on Sobol indices so as to identify the main inputs from a non-linear assessment model. The proposed methodology is illustrated through analysing sensitivity in an onshore wind and ground solar photovoltaic potential assessment covering two French regions. As a result, it is shown that, when estimating the potential of these renewable energy sources, parameters defining surface availability are more prevalent than those related to technology.

17/02177 Strategic bidding for price-maker producers in predominantly hydroelectric systems

Cruz, M. P. *et al. Electric Power Systems Research*, 2016, 140, 435–444.

This paper proposes an equilibrium model to determine price and quantity strategic bids for generation companies participating in a day-ahead electricity market, with predominantly hydroelectric generation. Each agent aims to maximize its profit by solving a bi-level optimization problem, where the upper level represents the producer revenue maximization problem, while the lower one consists of minimizing the cost of system operation, faced by the independent system operator. Price-maker companies operating both hydro and thermal plants are considered in a cascade hydro system with reservoirs managed by different owners. Consequently, a novel approach is proposed to decouple the first and second levels of the problem. The authors present an individual plant modelling, where the main constraints related to a hydrothermal system are considered. Through the utilization of the Karush–Kuhn–Tucker optimality conditions, the bi-level optimization model is converted to a single level non-linear problem, known in literature as a mathematical program with equilibrium constraints (MPEC). To face the difficulties of this non-linear, non-convex, multi-stage problem, the MPEC complementarity conditions are replaced by the strong duality condition. Moreover, competition among several leaders is modelled as an iterative procedure, and the methodology is applied in two systems with data and configurations derived from the Brazilian hydrothermal system.

17/02178 The benefits of flexibility: the value of wind energy with hydropower

Hirth, L. *Applied Energy*, 2016, 181, 210–223.

Several studies have shown that the revenue of wind power generators on spot markets ('market value') diminishes with increasing deployment. This 'value drop' is mostly observed in power markets that are dominated by thermal power plants, such as in Germany. This paper assesses the wind market value in power systems where hydroelectric stations with large reservoirs prevail, such as in Sweden. Due to their dispatch flexibility, such hydropower compensates for wind power output variability and thereby mitigates the wind power value drop. The market value of electricity from wind declines with penetration in both types of power systems, but it tends to decline at a slower rate if hydropower is present. This paper presents empirical evidence on the relevance of this effect derived from market data and numerical model results. The results indicate that when moving from 0% to 30% wind penetration, hydropower mitigates the value drop by a third. As a result, 1 MWh of wind energy is worth 18% more in Sweden than in Germany. Sensitivity analyses indicate high robustness despite large parameter uncertainty: in 80% of all sensitivities, wind energy is valuable 12–29% more in Sweden than in Germany. The benefits of hydropower seem to level off at around 20% wind penetration. This suggests that the hydro flexibility is 'exhausted' at this level. Low wind speed wind turbines, carbon pricing, and upgrades of hydropower generation capacity can lever the added value of hydro flexibility further. Not only is wind energy more valuable in the presence of hydropower, hydroelectricity also becomes more valuable if paired with wind power.

17/02179 The effects of yawing motion with different frequencies on the hydrodynamic performance of floating vertical-axis tidal current turbines

Wang, K. *et al. Applied Ocean Research*, 2016, 59, 224–235.

Under real sea conditions, the hydrodynamic performance of floating vertical-axis tidal current turbines is affected by waves and currents. The wave circular frequency is a significant factor in determining the frequencies of the wave-induced motion responses of turbines. In this study, the ANSYS-CFX software is used to analyse the hydrodynamic performance of a vertical-axis turbine for different yawing frequencies and to study how the yawing frequencies affect the main hydrodynamic coefficients of the turbine, including the power coefficient, thrust coefficient, lateral force coefficient, and yawing moment coefficient. The time-varying curves obtained from the CFX software are fitted using the least-squares method; the damping and added mass coefficients are then calculated to analyse the influence of different yawing frequencies. The simulation results demonstrate that when analysing non-yawing turbines rotating under constant inflow, the main hydrodynamic coefficient time-varying curves of yawing turbines exhibit an additional fluctuation. Furthermore, the amplitude is positively correlated with the yawing frequency, and the oscillation amplitudes also increase with increasing yawing frequency; however, the average values of the hydrodynamic coefficients (except the power coefficient) are only weakly influenced by yawing motion. The power coefficient under yawing motion is lower than that under non-yawing motion, which means that yawing motion will cause the annual energy production of a turbine to decrease. The fitting results show that the damping term and the added mass term exert effects of the same level on the loads and moments of vertical-axis turbines under yawing motion. The results of this study can facilitate the study of the motion response of floating vertical-axis tidal current turbine systems in waves.

17/02180 The importance of wave climate forecasting on the decision-making process for nearshore wave energy exploitation

López-Ruiz, A. *et al. Applied Energy*, 2016, 182, 191–203.

This work presents a new methodology for the medium- to long-term stochastic forecasting of the main variables and indexes related to the wave climate that are involved in the decision-making process to allocate, operate and maintain individual nearshore wave energy converters (WECs) and/or wave farms. Compared to the state-of-the-art approaches, this methodology includes the assessment of the uncertainty by means of Monte Carlo simulations, constituting a valuable step forward. The methodology is based on the simulation of N_y-year time series of wave climate variables that maintain the same statistical descriptors and seasonal and year-to-years variations of a hindcasted time series. This step is repeated N_e times to provide a sample size large enough to assess the uncertainty of the predictions. Because the wave energy resource is obtained from the nearshore, a large amount of wave propagations would be required. However, this methodology incorporates downscaling techniques that significantly improve the computational efficiency, and only a reduced number of N_w sea states should be propagated using an advanced numerical model. The methodology was applied to Playa Granada beach (southern Spain), obtaining the wave energy resource at 24 locations in the nearshore for 25-year time series repeated 1000 times. The selection of the most promising location for WECs on the basis of hindcasted or forecasted data provides different results. This highlights the importance of the proposed methodology for the advanced planning and design of any prospective energy extraction project.

17/02181 Towards 100% renewable energy systems: uncapping power system flexibility

Papaefthymiou, G. and Dragoon, K. *Energy Policy*, 2016, 92, 69–82.

This paper outlines the necessary steps to create power systems with the flexibility needed to maintain stability and reliability while relying primarily on variable energy resources. These steps are provided in the form of a comprehensive overview of policies, technical changes, and institutional systems, organized in three development phases: an initial phase (penetration up to about 10%) characterized by relatively mild changes to conventional power system operations and structures; a dynamic middle phase (up to about 50% penetration) characterized by phasing out conventional generation and a concerted effort to wring flexibility from existing infrastructure; and the high penetration phase that inevitably addresses how power systems operate over longer periods of weeks or months when variable generation will be in either short supply, or in over-abundance. Although this transition is likely a decades-long and incremental process and depends on the specifics of each system, the needed policies, research, demonstration projects and institutional changes need to start now precisely because of the complexity of the transformation. The list of policy actions presented in this paper can serve as a guideline to policy makers on effectuating the transition and on tracking the preparedness of systems.

17/02182 When energy policy meets community: rethinking risk perceptions of renewable energy in Germany and the Netherlands

Dóci, G. and Gotchev, B. *Energy Research & Social Science*, 2016, 22, 26–35.

Although in academic literature several analyses can be found concerning energy policy instruments and their effectiveness in supporting renewables, usually no distinction is made between different investor groups that these instruments address. The present

article focuses on an emerging group of investors, namely renewable energy communities, and on policy instruments fostering their operation and spread. The aim of the article is to assess and compare national support systems in Germany and in the Netherlands, respectively to identify which instruments are perceived as the ones most effectively supporting community-based renewable energy projects. To do so, first an investors' risk framework was adopted to evaluate the effectiveness of support systems according to their ability to decrease investors' risks, and this framework was operationalized by introducing indicators for a theory led analysis. Second, the investors' perceptions of the policy instruments were explored by conducting interviews with community members to see which instruments are perceived supportive in practice and which ones are less popular among community investors. The results show that in both countries instruments designed and expected to reduce specific types of risk do not always achieve that goal practice, and this is reflected in the perception of the aforementioned investor groups.

14 FUEL SCIENCE AND TECHNOLOGY

Fundamental science, analysis, instrumentation

17/02183 A framework for multi-stakeholder decision-making and conflict resolution

Dowling, A. W. *et al. Computers & Chemical Engineering*, 2016, 90, 136–150.

Here, the authors propose a decision-making framework to compute compromise solutions that balance conflicting priorities of multiple stakeholders on multiple objectives. In this setting, the authors shape the stakeholder dissatisfaction distribution by solving a conditional-value-at-risk (CVaR) minimization problem. The CVaR problem is parameterized by a probability level that shapes the tail of the dissatisfaction distribution. The proposed approach allows us to compute a family of compromise solutions and generalizes multi-stakeholder settings previously proposed in the literature that minimize average and worst-case dissatisfactions. The authors use the concept of the CVaR norm to give a geometric interpretation to this problem and use the properties of this norm to prove that the CVaR minimization problem yields Pareto optimal solutions for any choice of the probability level. A broad range of potential applications of the framework that involve complex decision-making processes are discussed. The authors also demonstrate the developments using a biowaste facility location case study, which seeks to balance stakeholder priorities on transportation, safety, water quality, and capital costs.

17/02184 A game theory approach to vulnerability analysis: integrating power flows with topological analysis

Cheng, M. X. *et al. International Journal of Electrical Power & Energy Systems*, 2016, 82, 29–36.

This paper presents a new framework for vulnerability analysis. Under this framework, the authors were able to identify the vulnerable components and the critical components of a power grid. Distinct from previous work, this model considers the interaction between the components of the power system, and models the dynamic evolving process of cascading failures. The impact of a component failure on the system is dynamically changing as the failure propagates. The authors analyse the vulnerability of a power grid using an optimization model based on game theory, and use linear programming method to solve it. Since instability is the reason of power outage, an instability index was used to measure the negative impact to the system. The results from this optimization problem suggest which component of the system is critical since its failure can most negatively impact the cyber-physical system.

17/02185 Augmentation of transient stability margin based on rapid assessment of rate of change of kinetic energy

Al-Taee, A. A. *et al. Electric Power Systems Research*, 2016, 140, 588–596.

A fast-load injection through a resistive dynamic brake with appropriate power dissipation capacity can absorb the excess transient energy caused by a large and sudden disturbance and thus improve the transient stability margin of a power system. However, fast assessment of the transient stability and the effective insertion/removal instants of the brake are longstanding challenges. This paper proposes a new criterion based on the rate of change of kinetic energy to rapidly evaluate system transient stability and identify conditions of effective insertion/removal instants of a dynamic brake. Unlike reported studies where the superiority of this criterion was only demonstrated through off-line simulation, both the theoretical modelling and practical implementation of this criterion is presented here using the one machine infinite bus system. A microprocessor controller based on a single-variable measurement, i.e. generator deviation speed, is proposed and implemented to control the dynamic brake during the disturbance periods. The observed behaviour of the power system under sudden disturbances and the effect of timely insertion/removal of the dynamic brake on the transient stability of the power system under study are presented and evaluated. The proposed method has been successfully validated, demonstrating its suitability for practical and rapid assessment of transient stability.

17/02186 Calling for change? Innovation, diffusion, and the energy impacts of global mobile telephony

Bento, N. *Energy Research & Social Science*, 2016, 21, 84–100.

Few technologies in history diffused as intensively and fast as mobile phones, to the point where they have become the most democratic technology. The article analyses historical patterns of mobile phone growth and their effects in energy needs. Through an empirical analysis employing diffusion models on data for 227 countries between 1980 and 2010, it is concluded that global demand may saturate at around one subscription per person and the diffusion of mobile-broadband connection has contributed to sustain growth. Demand has already showed signs of saturation in developed countries, while there is still potential for growth in developing countries. Impacts on energy consumption are assessed with the help of a field trial. Even though the energy consumed in phone charging was not very significant (6–8 TWh) in 2010, it becomes substantially higher when infrastructural needs are included (93 TWh). The actual trends suggest that mobile communication might have a sizeable direct effect on energy consumption – although the net impact on energy demand is more difficult to estimate. This can become an issue in developing countries, where the adoption of mobile phones is catching-up rapidly with the world average, in a context of generalized increasing electricity demand.

17/02187 Characterization of cell wall structure in dilute acid-pretreated biomass by confocal Raman microscopy and enzymatic hydrolysis

Na, B.-I. *et al. Biomass and Bioenergy*, 2016, 93, 33–37.

The chemical and ultrastructural properties of cell walls were investigated to determine the effect of dilute acid pretreatment on the hydrolysis of lignocellulosic biomass. Confocal Raman microscopy was used to gain a clear understanding of how dilute acid pretreatments destroy lignocellulosic cell walls. Total fermentable sugar (glucose and xylose) was high in oxalic acid hydrolysate (26.18 g/L) compared to that in sulfuric acid hydrolysate (24.34 g/L). Chemical composition of the pretreated biomass differed slightly according to the acid catalyst used. Oxalic acid pretreatment was effective for enzymatic hydrolysis, with 29.46 g/L of total fermentable sugar after 96 h. Optical microscopy showed that dilute acid pretreatment significantly changed the cell wall structure, and broken and crushed cell walls could be clearly seen during pretreatment. Based on confocal Raman peak intensity, the ratio of lignin/cellulose [I(1600)/I(900)] was low for oxalic acid-pretreated biomass compared to sulfuric acid-pretreated biomass.

17/02188 Comparison of Raman and IR spectroscopy for quantitative analysis of gasoline/ethanol blends

Corsetti, S. *et al. Fuel*, 2016, 166, 488–494.

Ethanol is commonly admixed to petrochemical gasoline, and its amount in the fuel blend can influence the performance of an engine. The ethanol content in a commercial fuel can vary. To ensure reliable engine operation, control strategies based on a measurement of the composition need to be developed. Two possible methods to determine the ethanol content in ethanol/gasoline blends are Raman and IR spectroscopy. The authors compared both techniques for quantitative measurements in systematically varied blends of ethanol and a gasoline surrogate. For each method, two different approaches for data evaluation were tested and compared: Firstly, the calibration of the intensity ratio of characteristic peaks as function of composition; secondly, a principal component regression (PCR). Both methods were found to have comparable uncertainty. For the evaluation of the Raman spectra, the PCR method yielded better accuracy than the intensity ratio approach. In addition, a detailed investigation of the influence of noise in the signal is presented. When the full IR spectra were evaluated by PCR, even high noise levels did not reduce the measurement accuracy significantly.

17/02189 Computer code ENDSAM for random sampling and validation of the resonance parameters covariance matrices of some major nuclear data libraries

Plevnik, L. and Žerovnik, G. *Annals of Nuclear Energy*, 2016, 94, 510–517.

Methods for random sampling of correlated parameters are presented. The methods are implemented for sampling of resonance parameters in ENDF-6 format and a link to the open-source code ENDSAM is given. The code has been validated on realistic data. Additionally, consistency of covariances of resonance parameters of three major contemporary nuclear data libraries (JEFF-3.2, ENDF/B-VII.1 and JENDL-4.0u2) has been checked.

17/02190 Design and development of a helium injection system to improve external leakage detection during liquid nitrogen immersion tests

Townsend, A. and Mishra, R. *Cryogenics*, 2016, 79, 17–25.

The testing of assemblies for use in cryogenic systems commonly includes evaluation at or near operating (therefore cryogenic) temperature. Typical assemblies include valves and pumps for use in liquid oxygen–liquid hydrogen rocket engines. One frequently specified method of cryogenic external leakage testing requires the assembly, pressurized with gaseous helium (GHe), be immersed in a bath of liquid nitrogen (LN_2) and allowed to thermally stabilize. Component interfaces are then visually inspected for leakage (bubbles). Unfortunately the liquid nitrogen will be boiling under normal, bench-top, test conditions. This boiling tends to mask even significant leakage. One little known and perhaps under-utilized property of helium is the seemingly counter-intuitive thermodynamic property that when ambient temperature helium is bubbled through boiling LN_2 at a temperature of $-195.8\,^{\circ}C$, the temperature of the liquid nitrogen will reduce. This paper reports on the design and testing of a novel proof-of-concept helium injection control system confirming that it is possible to reduce the temperature of an LN_2 bath below boiling point through the controlled injection of ambient temperature gaseous helium and then to efficiently maintain a reduced helium flow rate to maintain a stabilized liquid temperature, enabling clear visual observation of components immersed within the LN_2. Helium saturation testing is performed and injection system sizing is discussed.

17/02191 Development of fuel composition measurement technology using laser diagnostics

Kamimoto, T. *et al. Applied Thermal Engineering*, 2016, 102, 596–603.

The purpose of this research is the development of real-time fuel composition measurement technology using laser diagnostics. In recent years, gas turbine combustors have used a diversity of fuels and the diversification of fuel requires the advanced combustion control technologies. By monitoring fuel gas compositions in real time, optimal fuel compositions can be prepared and applied to the gas turbine operations. The active control using measurement results of gas compositions results in combustion stability and the reduction of environmental pollutants. In this study, the real-time measurement equipment of fuel gas compositions was developed using Raman spectroscopy and tunable diode laser absorption spectroscopy (TDLAS). The colinear optical configuration using Raman spectroscopy was newly employed to enhance the signal intensity and stability of the system. It was demonstrated that it detected the composition of gas turbine fuels within 2 s using Raman spectroscopy and 0.3 s using TDLAS within the relative standard deviations of 1–3%. It also showed the robustness to fine particles in gases, which has proved its applicability to actual gas turbines. The developed system was applied to a 300 MW commercial gas turbine combustor to monitor the fuel gas composition and gas heating value and showed the 240 s faster response time to the conventional gas chromatography method.

17/02192 Drone with thermal infrared camera provides high resolution georeferenced imagery of the Waikite geothermal area, New Zealand

Harvey, M. C. *et al. Journal of Volcanology and Geothermal Research*, 2016, 325, 61–69.

Drones are now routinely used for collecting aerial imagery and creating digital elevation models (DEM). Lightweight thermal sensors provide another payload option for generation of very high-resolution aerial thermal orthophotos. This technology allows for the rapid and safe survey of thermal areas, often present in inaccessible or dangerous terrain. Here the authors present a $2.2\,km^2$ georeferenced, temperature-calibrated thermal orthophoto of the Waikite geothermal area, New Zealand. The image represents a mosaic of nearly 6000 thermal images captured by drone over a period of about 2 weeks. This is thought by the authors to be the first such image published of a significant geothermal area produced by a drone equipped with a thermal camera. Temperature calibration of the image allowed calculation of heat loss (43 ± 12 MW) from thermal lakes and streams in the survey area (loss from evaporation, conduction and radiation). An RGB (visible spectrum) orthomosaic photo and digital elevation model was also produced for this area, with ground resolution and horizontal position error comparable to commercially produced LiDAR and aerial imagery obtained from crewed aircraft. The results show that thermal imagery collected by drones has the potential to become a key tool in geothermal science, including geological, geochemical and geophysical surveys, environmental baseline and monitoring studies, geotechnical studies and civil works.

17/02193 Effect of reciprocating motions around working points on levitation force of superconductor-magnet system

Xu, J. *et al. Cryogenics*, 2016, 78, 96–102.

In order to simulate vibration around working points in practical operation of superconducting levitation system, magnet in a simple superconductor-magnet system are conducted reciprocating motions around static height in this study. Two YBCO cylindrical samples with different grain orientations are used to investigate the effect of reciprocating motions of magnet on superconducting magnetic force. The *c*-axis of sample S1 is perpendicular to the top surface while sample S2 is parallel to the top surface. The initial cooling processes for the superconductors include zero-field-cooled (ZFC) and filed-cooled (FC). Compared to the levitation force before reciprocating motions, the ZFC levitation force at static height becomes smaller after reciprocating while the FC force presents opposite phenomenon. It is found that levitation force at static height tends to be stable after several times of reciprocating under ZFC and FC conditions and its time-decay phenomenon is suppressed in some extent, which is meaningful for the practical application of superconducting levitation system. Based on vortex dynamic, some physical discussions are presented to the experimental results.

17/02194 Effect of superficial gas velocity on the particle temperature distribution in a fluidized bed with heat production

Li, Z. *et al. Chemical Engineering Science*, 2016, 140, 279–290.

The heat transfer behaviour of particles and gas in an olefin polymerization fluidized bed was numerically analysed using an in-house developed 3-D computational fluid dynamics discrete element model (CFD-DEM). First the implementation of the model was verified by comparing simulation results with analytical results. A constant volumetric heat production rate was implemented in the particle energy equation to mimic the heat production due to the polymerization reaction. It was found that the probability density function (PDF) of the particle temperature becomes more homogeneous with increasing superficial gas velocity. Furthermore, instantaneous snapshots of the thermal driving force (the difference between the single particle temperature and bed-average gas temperature, $T_p - T_g$) for different heat production rates provide detailed insight in the particle temperature distribution inside the fluidized bed. The time- and bed-averaged particle convective heat transfer coefficient, which was calculated by Gunn's correlation, was found to be independent of the superficial gas velocity. This is explained by the fact that the relative velocity of gas and particles in the emulsion phase, where most of the particles and gas interact, is hardly influenced when increasing the gas superficial velocity. From the spatial distribution of Nusselt number, it becomes apparent that the high heat transfer regions are found in the wake of rising bubbles, whereas low heat transfer rates are found in the clouds of the bubbles.

17/02195 Energetic optimization of regenerative braking for high speed railway systems

Frilli, A. *et al. Energy Conversion and Management*, 2016, 129, 200–215.

The current development trend in the railway field has led to an ever increasing interest for the energetic optimization of railway systems (especially considering the braking phases), with a strong attention to the mutual interactions between the loads represented by railway vehicles and the electrical infrastructure, including all the sub-systems related to distribution and smart energy management such as energy storage systems. In this research work, the authors developed an innovative coupled modelling approach suitable for the analysis of the energetic optimization of railway systems and based on the use of the new object oriented language Matlab-Simscape, which presents several advantages with respect to conventional modelling tools. The proposed model has been validated considering an Italian direct current high-speed line and the high-speed train ETR 1000. Furthermore, the model has been used to perform an efficiency analysis, considering the use of energy storage devices. The results obtained with the developed model show that the use of energy recovery systems in high-speed railway can provide great opportunities of energy savings.

17/02196 Explaining the historical energy use in dwelling stocks with a segmented dynamic model: case study of Norway 1960–2015

Sandberg, N. H. *et al. Energy and Buildings*, 2016, 132, 141–153.

A segmented dynamic dwelling stock model is proven useful for understanding the development and changes of ageing building stocks, which is highly relevant for renovation measures and estimates of energy use and emissions in aggregated building stocks. In this paper, such a model is developed further for detailed analyses of dwelling stock energy demand and exemplified for the Norwegian dwelling stock 1960–2015. The dwelling stock model simulates the development in stock size and composition and is combined with archetype-specific energy intensities to estimate the total energy demand. After calibrating the model results with statistics, the model is used to explore the phenomena and causes of historical changes. A large-scale improvement of the energy efficiency of the Norwegian dwelling stock has taken place through renovation and construction of new dwellings. A historical shift to more efficient energy carriers and heating systems has had an effect on energy savings in the system, of the same size as the effect of the improved energy efficiency of the stock. However, the total average energy savings per m^2 are offset by changes in user heating habits. A significant decrease in average delivered energy intensity per m^2 is only observed after the introduction of heat pumps.

17/02197 Forced flow He vapor cooled critical current testing facility for measurements of superconductors in a wide temperature and magnetic field range

Baskys, A. *et al. Cryogenics*, 2016, 79, 1–6.

As superconducting materials find their way into applications, there is increasing need to verify their performance at operating conditions. Testing of critical current with respect to temperature and magnetic field is of particular importance. However, testing facilities covering a range of temperatures and magnetic fields can be costly, especially when considering the cooling power required in the cryogenic system in the temperature range below 65 K (inaccessible for LN_2). Critical currents in excess of 500 A are common for commercial samples, making the testing of such samples difficult in setups cooled via a cryocooler, moreover it often does not represent the actual cooling conditions that the sample will experience in service. This work reports the design and operation of a low-cost critical current testing facility, capable of testing samples in a temperature range of 10–65 K, with magnetic field up to 1.6 T and measuring critical currents up to 900 A with variable cooling power.

17/02198 Geochemical and flow modelling as tools in monitoring managed aquifer recharge

Niinikoski, P. *et al. Applied Geochemistry*, 2016, 74, 33–43.

Due to a growing world population and the effects of anthropogenic climate change, access to clean water is a growing global concern. Managed aquifer recharge (MAR) is a method that can help society's response to this increasing demand for pure water. In MAR, the groundwater resources are replenished and the quality of the recharged surface water is improved through effects such as the removal of organic matter. This removal occurs through mechanisms such as microbial decomposition, which can be monitored by studying the isotopic composition of dissolved inorganic carbon (DIC). Nevertheless, the monitoring can be difficult when there are other factors, like dissolving calcite, affecting the isotopic composition of DIC. The aims of this study were to establish a method for monitoring the decomposition of organic matter (dissolved organic carbon – DOC) in cases where calcite dissolution adds another component to the DIC pool, and to use this method to monitor the beginning and amount of DOC decomposition on a MAR site at Virttaankangas, south-western Finland. To achieve this, the authors calculated the mean residence times of infiltrated water in the aquifer and the fractions of this water reaching observation wells. They also conducted geochemical modelling, using PHREEQC, to estimate the amount of DOC decomposition and the mineral reactions affecting the quality of the water.

17/02199 Investigation of bubble dynamics of underwater explosion based on improved compressible numerical model

Xiao, W. *et al. Applied Ocean Research*, 2016, 59, 472–482.

A bubble jet with velocity of hundred meters per second forms at the final stage of bubble collapse, which makes the compressibility of flow field cannot ignore. Based on the spherical bubble model of Geers and Hunter, a compressible numerical model is improved for simulating non-spherical bubble dynamic in this paper. In this implementation, the compressibility of external liquid and the wave effect of internal gas are considered by the first order external doubly asymptotic approximation and the first-order internal doubly asymptotic approximation, respectively. In addition, the volume acceleration model is applied to calculate the initial condition of bubble. After that, the improved compressible numerical model is validated against the underwater explosion experiment data. The numerical result of bubble radius correlates well with the experiment data. Finally, based on the improved compressible numerical model, the influences of wave effect of internal gas and initial condition of bubble on bubble dynamics in free field and gravity field are investigated. The wave effect of internal gas makes bubble radius, radial velocity, translational displacement, jet velocity and remaining total energy decrease. The initial radial velocity, on the one hand, makes bubble radius, radial velocity, translational displacement, jet velocity and remaining total energy increase at the first bubble cycle; on the other hand, intensifies bubble radius, radial velocity, translational displacement, jet velocity and remaining total energy decay.

17/02200 Liquid sloshing in partly-filled laterally-excited cylindrical tanks equipped with multi baffles

Wang, W. *et al. Applied Ocean Research*, 2016, 59, 543–563.

Baffles are used effectively to reduce the sloshing response of liquid in the liquid storage containers. This study is aimed at analysis of transient lateral sloshing in a partially-filled cylindrical tank with multi baffles including floating circular baffle, wall-mounted ring baffle, floating ring baffle and their combination form, and those baffles with inclination using a coupled multimodal method and scaled boundary finite element method (SBFEM). Slosh frequencies and mode shapes are initially estimated using the extending semi-analytical SBFEM by applying the linearized free surface boundary condition using the zoning method, where the liquid domain is firstly divided into several simple sub-domains so that the liquid velocity potential in each sub-domain has continuous boundary conditions of class C^1. As a key point, a new type of local co-ordinate system for SBFEM with axisymmetric geometry is presented for each sub-domain. Based on the multimodal method, significant improvement in computational time is achieved by reducing the generalized eigenvalue problem to a standard one involving only the velocity potentials on the two-dimensional half free-surface length. The generalized coordinates of the free-surface oscillations under a lateral excitation are then obtained from superposition of the natural slosh modes. The sloshing mass and lateral slosh force are also formulated in terms of the generalized coordinates and hydrodynamic coefficients. The validity of the model is examined through comparisons with available other solutions, and the results show that the present method has higher accuracy and efficiency with a very small number of degrees of freedom for the simulation of the complex sloshing problem partly-filled laterally-excited cylindrical tanks. It is also shown that consideration of only the first sloshing mass is adequate to represent the dynamic behaviour of the liquid container quite accurately. The effects of liquid fill level, baffled arrangement and length of those baffles upon the sloshing masses and sloshing forces are discussed in detail.

17/02201 Mass transfer and gas–liquid interface properties of single CO_2 bubbles rising in tap water

Nock, W. J. *et al. Chemical Engineering Science*, 2016, 140, 171–176.

To improve the mass transfer efficiency in many industrial applications better understanding of the mass transfer rate is required. High-speed images of single CO_2 bubbles rising in tap water were analysed to investigate the relationship between the mass transfer and properties of single bubbles. Transition to a lower mass transfer rate was shown to correspond with the transition from a mobile to an immobile bubble surface. This was indicated by the change in bubble rise velocity, bubble rise path and bubble shape. The presence of surfactants in untreated tap water appear to effect the transition point, particularly for bubbles with a smaller initial diameter and lower rise velocity.

17/02202 Modeling energy conversion in a tortuous stack for thermoacostic applications

Dragonetti, R. *et al. Applied Thermal Engineering*, 2016, 103, 233–242.

The stack represents the core of standing wave engines since inside it the thermal energy is converted into mechanical energy. Commonly stacks are realized with straight pores whose sections have regular shapes (e.g. circular, rectangular). In these cases the viscous and thermal interactions are described by well-known spatially averaged thermal and viscous functions. Instead, for a materials having tortuous pore, there is a lack in theoretical description of the thermoacoustic phenomenon. This paper deals with the performance of a thermoacoustic engine in which a tortuous porous material is used as stack. The spatially averaged thermal and viscous functions are obtained by classical models used to describe the sound propagation inside a porous material. In particular the Johnson–Champoux–Allard model is considered. It requires the knowledge of five parameters instead of the only hydraulic radius used to describe the standard stack having straight pores (e.g. circular, slit or square pores). The physical meaning of these parameters is explained starting from a straight circular pore and modifying, step by step, the shape of the pore until it becomes tortuous. The proposed functions have been included in the Rott theory and implemented in a numerical procedure. The achieved results are useful to analyse the thermoacoustic performance of a standing wave engine and to understand how the gain factor as well as the viscous and thermal losses inside the stack are affected by the tortuosity. A validation of this procedure is given by comparing the obtained results with ones given by DeltaEC software. This work can be

useful to understand the applicability of tortuous porous materials, such as fibrous material as well as open-cell material, for standing wave thermoacoustic engines.

17/02203 Spin test of three-dimensional composite rotor for flywheel energy storage system

Hiroshima, N. *et al. Composite Structures*, 2016, 136, 626–634.

A rotating disk often undergoes severe vibration at high rotation speeds because of unstable joining between the disk and a drive shaft. As described here, three connection methods between a driving shaft and an annular rotation disk made of three-dimensionally carbon-fibre reinforced composite were discussed to achieve stable rotation at high rotation speeds by changing the hub material and joining geometry: the connecting device. In two of the three methods, the vibration amplitude increased at a tip speed higher than 500 m/s. Key factors that caused the vibration were analysed. Results show that the third method by which a resin ring (hub) was inserted between the disk and rotation shaft maintained stable joining, even at high-speed rotation.

17/02204 Study on multi-fractal fault diagnosis based on EMD fusion in hydraulic engineering

Lu, S. *et al. Applied Thermal Engineering*, 2016, 103, 798–806.

The vibration signal analysis of the hydraulic turbine unit aims at extracting the characteristic information of the unit vibration. The effective signal processing and information extraction are the key to state monitoring and fault diagnosis of the hydraulic turbine unit. In this paper, the vibration fault diagnosis model is established, which combines empirical mode decomposition (EMD), multi-fractal spectrum and modified BP neural network; the vibration signal waveform is identified and purified with EMD to obtain approximation coefficient of various fault signals; the characteristic vector of the vibration fault is acquired with the multi-fractal spectrum algorithm, which is classified and identified as input vector of BP neural network. The signal characteristics are extracted through the waveform, the diagnosis and identification are carried out in combination of the multi-fractal spectrum to provide a new method for fault diagnosis of the hydraulic turbine unit. After the application test, the results show that the method can improve the intelligence and humanization of diagnosis, enhance the man–machine interaction, and produce satisfactory identification result.

17/02205 Textile energy storage: structural design concepts, material selection and future perspectives

Zhai, S. *et al. Energy Storage Materials*, 2016, 3, 123–139.

As a crucial element of human civilization, textiles reflect the range of materials indispensable for a variety of fundamental technologies that had been mastered throughout the history. In recent years, textiles are in a growing research frontier where fabrics and yarns can directly serve as electrical energy storage devices by themselves to develop wearable energy solutions. Integrated textile energy storage devices may power new functions, such as sensing, therapy, navigation, and communication, while preserving good wearability similar to original textiles. In this review, the authors introduce the design concepts and structures of textile energy storage devices currently explored including fabrication approaches. They particularly highlight key findings of creating two-dimensional textile and one-dimensional yarn supercapacitors and batteries. Critically, the challenges for future research development were discussed and the authors presented their perspectives. It is hoped that this paper stimulates further research into creating textile energy storage devices for wide practical applications.

17/02206 Three powerful nature-inspired algorithms to optimize power flow in Algeria's Adrar power system

Makhloufi, S. *et al. Energy*, 2016, 116, 1117–1130.

This paper is intended to solve the optimal power flow (OPF) dispatch in the presence of wind power generation (WPG) in the Adrar power system. Towards this aim, the performances of three powerful metaheuristic algorithms-namely, the cuckoo search algorithm (CSA), firefly algorithm (FFA), and flower pollination algorithm (FPA) are investigated. The proposed algorithms are applied to best capture the active power produced with the minimum value of a multi-objective function. This latter includes: the fuel cost, the NOx emissions, and the imbalance cost of the WPGs. Furthermore, considering the uncertainties governing wind resources, the maximum wind power output is estimated using the wind speed carrying maximum energy. It was found that all algorithms perform well in providing accurate solutions. Interestingly, the convergence is reached in the first 135 iterations. A remarkable outcome of the present work is that CSA outperforms FPA and FFA. CSA has proved itself to be a great tool to optimize Adrar's power flow system in term of iterations and computational time.

17/02207 Utilising light-emitting diodes of specific narrow wavelengths for the optimization and co-production of multiple high-value compounds in *Porphyridium purpureum*

Coward, T. *et al. Bioresource Technology*, 2016, 221, 607–615.

The effect of specific narrow light-emitting diode (LED) wavelengths (red, green, blue) and a combination of LED wavelengths (red, green and blue – RGB) on biomass composition produced by *Porphyridium purpureum* is studied. Phycobiliprotein, fatty acids, exopolysaccharides, pigment content, and the main macromolecules composition were analysed to determine the effect of wavelength on multiple compounds of commercial interest. The results demonstrate that green light plays a significant role in the growth of rhodophyta, due to phycobiliproteins being able to harvest green wavelengths where chlorophyll pigments absorb poorly. However, under multi-chromatic LED wavelengths, *P. purpureum* biomass accumulated the highest yield of valuable products such as eicosapentaenoic acid (~2.9% DW), zeaxanthin (~586 $\mu g\,g^{-1}$ DW), β-carotene (397 $\mu g\,g^{-1}$ DW), exopolysaccharides (2.05 g/L^{-1}), and phycobiliproteins (~4.8% DW). This increased accumulation is likely to be the combination of both photo-adaption and photo-protection, under the combined specific wavelengths employed.

17/02208 Wearable thermoelectric generators for human body heat harvesting

Hyland, M. *et al. Applied Energy*, 2016, 182, 518–524.

A thermoelectric generator (TEG) can be used to harvest electrical energy from human body heat for the purpose of powering wearable electronics. At the NSF Advanced Self-powered Systems of Integrated Sensors and Technologies (ASSIST), TEGs are one of the enabling technologies being explored to advance the centre's mission of creating wearable, self-powered, health and environmental monitoring systems. As part of this effort, an exploration of the relevant parameters for maximizing the wearable TEG power output from the body heat and maintaining the body comfort is particularly important. For this purpose, the heat from the body must be directed into TEG with minimal loss, the generator must be designed for maintaining a high temperature differential across the thermoelectric material, and the generator must have a small form factor to maintain the body comfort. In order to address these requirements, an optimum TEG design was developed and experiments were conducted both on a temperature-controlled hot plate and on different body locations including the wrist, upper arm, and chest. The TEG was further fabricated into a T-shirt and the power was recorded for different human activities. Comparison of the experiments on various body locations and on the T-shirt yielded the highest to lowest power generated on the upper arm, wrist, chest and T-shirt, respectively. The prospect of powering a wearable electrocardiogram sensor by a TEG on the upper arm is discussed.

Fuel cell technology

17/02209 An improved ethanol microfluidic fuel cell based on a PdAg/MWCNT catalyst synthesized by the reverse micelles method

Armenta-González, A. J. *et al. Fuel*, 2016, 167, 240–247.

In this work, two electrocatalysts based on Pd (Pd/MWCNT and PdAg/MWCNT) were synthesized using reverse micelles for ethanol oxidation (EOR), and evaluated in an air-breathing microfluidic fuel cell. Commercial Pd (Pd/C) was used for comparison. The average nanoparticle size estimated by TEM was approximately 4–7 nm for both electrocatalysts. TGA measurements indicated that the electrocatalysts had similar metallic loading (19% for Pd and 17% for PdAg). The materials were tested for EOR in 1 M KOH. Fuel cell tests were performed in an air-breathing microfluidic fuel cell (ABμFFC) in which oxygen was obtained from the air to improve the performance of the cathodic reaction. The results were compared with those obtained using a closed microfluidic fuel cell (μFFC). In these devices, two streams were injected, one containing fuel and the other containing an electrolyte solution (1 M KOH), and commercial Pt (Pt/C) was used as cathodic catalyst. The ABμFFC that used the PdAg/MWCNT electrocatalyst performed better (almost 70% more power was harvested) than the one that used the Pd/MWCNT electrocatalyst. Finally, the power density harvested from the ABμFFC was four times higher than that harvested from the μFFC.

17/02210 Atomic layer deposition of yttria-stabilized zirconia thin films for enhanced reactivity and stability of solid oxide fuel cells

Park, J. *et al. Energy*, 2016, 116, 170–176.

This paper reports the advantages of atomic layer deposition (ALD) for the fabrication of yttria-stabilized zirconia (YSZ) electrolyte. The reactivity and stability of anodic aluminium oxide (AAO)-based thin-film solid oxide fuel cells (SOFCs) are improved by applying ALD YSZ electrolyte. The fuel cell fabricated by ALD shows a peak power density of 154.6 $mW\,cm^{-2}$ at 450 °C, whereas the fuel cell fabricated by sputtering demonstrates a peak power density of 66.2 $mW\,cm^{-2}$. The

amorphous and nanogranular microstructure of the ALD YSZ film is ascribed for a significant improvement in the cathodic reactivity of the AAO-based thin-film fuel cells. Moreover, the smooth and uniform surface of the ALD YSZ electrolytes mitigates the agglomeration of the Pt cathode layer, and thus the thermal stability of the thin-film fuel cell is remarkably improved at 450 °C.

17/02211 Biofouling inhibition and enhancing performance of microbial fuel cell using silver nano-particles as fungicide and cathode catalyst

Noori, M. T. *et al. Bioresource Technology*, 2016, 220, 183–189.

Morphological analysis of biofouling developed on cathode surface in an air-cathode microbial fuel cell (MFC) was performed. For sustaining power production and enhancing Coulombic efficiency (CE) of MFC, studies were conducted to inhibit cathode biofouling using different loadings of silver nanoparticles (Ag-NPs) with 5% and 10% Ag in carbon black powder. In MFC without using Ag-NPs in cathode (MFC-C), cathode biofouling increased the charge transfer resistance (R_{ct}) from 1710 to 2409 $\Omega\,cm^2$, and reduced CE by 32%; whereas in MFC with 10% Ag in cathode R_{ct} increased by only 5%. Power density of $7.9 \pm 0.5\,W/m^3$ in MFC using 5% Ag and $9.8 \pm 0.3\,W/m^3$ in MFC using 10% Ag in cathode was 4.6 and 5.7 times higher than MFC-C. These results suggest that the Ag-NPs effectively inhibit the fungal biofouling on cathode surface of MFCs and enhanced the power recovery and CE by improving cathode kinetics.

17/02212 Development, analysis and assessment of a fuel cell and solar photovoltaic system powered vehicle

Ezzat, M. F. and Dincer, I. *Energy Conversion and Management*, 2016, 129, 284–292.

This paper deals with a new hybrid-powered photovoltaic–fuel cell–Li-ion battery integrated system and is compared to a base system, consisting of proton exchange membrane fuel cell and Li-ion battery. It investigates the effects of adding photovoltaic arrays to the base system and further effects on the overall energy and exergy efficiencies and hence hydrogen consumption. These two systems are analysed and assessed both energetically and exergetically. The study results show that the overall energy and exergy efficiencies become 39.46% and 56.3%, respectively at a current density of 1150 mA/cm^2 for system 1 (fuel cell–battery). Moreover, energy and exergy efficiencies are found to be 39.86% and 56.63% at current density of 1150 mA/cm^2 for system 2 (fuel cell–battery–photovoltaics). Utilizing photovoltaic arrays in system 2 would recover 561 g of hydrogen through 3 h of continuous driving at max power of 98.32 kW, which is approximately 11.2% of the hydrogen storage tank used in the proposed systems. The effects of changing various system parameters on energy and exergy efficiencies of the overall system are also examined.

17/02213 Effect of reverse Boudouard reaction catalyst on the performance of solid oxide carbon fuel cells integrated with a dry gasifier

Kim, S.-K. *et al. Energy Conversion and Management*, 2016, 130, 119–129.

A solid oxide carbon fuel cell (SO-CFC) integrated with a dry gasifier was operated on activated carbon fuel and the effect of adding a reverse Boudouard gasification catalyst on the performance and long-term operation characteristics of the SO-CFC was investigated. The reactivity of the carbon fuels for the Boudouard gasification reaction was analysed by a thermal analysis at various operating conditions. The SO-CFC was then operated on gasified fuel gas consisting of CO_2 and CO obtained from the integrated dry gasifier. The SO-CFC operated on activated carbon fuel with 5 wt% K_2CO_3 achieved a maximum power density of 202, 262 and 271 mW/cm^2 at 750, 800 and 850 °C, respectively; the SO-CFC fuelled with activated carbon fuel without a catalyst meanwhile yielded maximum power density of 168 mW/cm^2 at 850 °C. By using electrochemical impedance spectroscopy, the effect of adding the catalyst on the gasification products and subsequently on the performance of the SO-CFC was studied. A long-term degradation test was conducted by continuously operating the SO-CFC at 50 mA/cm^2 for 518 h at 750 °C. During the long-term degradation test, the average degradation rate of the SO-CFC was found to be 183 mV/kh. The *post-mortem* scanning electron microscopy and X-ray diffraction analyses of the SO-CFC after the long-term test revealed the presence of carbon deposits and oxidation of Ni at the anode, causing a relatively higher degree of degradation in the SO-CFC integrated with the dry gasifier during the long-term operation. The addition of the K_2CO_3 based dry gasification catalyst significantly enhances the performance of the SO-CFC integrated with dry gasification, but during long-term operation, the degradation rate is found to be higher than that of conventional H_2 fuelled solid oxide fuel cells.

17/02214 Efficiency analysis of a hydrogen-fueled solid oxide fuel cell system with anode off-gas recirculation

Peters, R. *et al. Journal of Power Sources*, 2016, 328, 105–113.

This study analyses different hydrogen-fuelled solid oxide fuel cell (SOFC) system layouts. It begins with a simple system layout without any anode off-gas recirculation, continues with a configuration equipped with off-gas recirculation, including steam condensation and then considers a layout with a dead-end anode off-gas loop. Operational parameters such as stack fuel utilization, as well as the recirculation rate, are modified, with the aim of achieving the highest efficiency values. Drawing on experiments and the accumulated experience of the SOFC group at the Forschungszentrum Jülich, a set of operational parameters were defined and applied to the simulations. It was found that anode off-gas recirculation, including steam condensation, improves electrical efficiency by up to 11.9 percentage-points compared to a layout without recirculation of the same stack fuel utilization. A system layout with a dead-end anode off-gas loop was also found to be capable of reaching electrical efficiencies of more than 61%.

17/02215 Efficient microscale simulation of intermediate-temperature solid oxide fuel cells based on the electrochemical effectiveness concept

Shin, D. *et al. Computers & Chemical Engineering*, 2016, 90, 268–277.

In this study, a new microscale simulation method based on the electrochemical effectiveness concept is proposed for efficient calculation of intermediate-temperature solid oxide fuel cells (IT-SOFCs). The electrochemical effectiveness model can accurately determine the current generation efficiencies of thin active functional layers in IT-SOFC electrodes, without the need to place many grid points and solve complex electrochemical reaction/charge transport equations. Thus, the effectiveness-based microscale simulation method is developed by modifying a previous microscale model to include the effectiveness model formulation, and the simulation results for one-dimensional, single-cell performances of IT-SOFCs are compared with the results from the microscale models. The proposed microscale simulation method is shown to accurately reproduce the results of more detailed calculations at much lower computational costs, which suggests that the present method can be useful for developing large-scale simulation models for IT-SOFCs.

17/02216 Impact of fuel cell and battery size to overall system performance – a diesel fuel-cell APU case study

Pregelj, B. *et al. Applied Energy*, 2016, 182, 365–375.

In this paper a data-validated power-efficiency model of a diesel-powered fuel-cell-based auxiliary power unit (APU) system is used to investigate the various sizes of the power unit and the battery and to evaluate the optimal choices for specified load profiles. The challenge comes from the fuel cell-based power generation (FCGEN) EU FP7 project, where such an APU was developed. The system consists of a fuel processor, a polymer electrolyte membrane stack, and a battery providing power for the start-up, shutdown, and for covering load transients; however, the developed prototype system is not optimized. Before redesigning it for mass production, the optimal size of the main components needs to be identified to enable the best possible exploitation of the technology. In this work a case-specific load profile was used and a mesh grid of scenario simulations has been performed using various sizes of the fuel cell with fuel processor as a power unit and the batteries of various capacities as an energy storage unit. For this purpose a scalable APU model, including the BoP component consumption, has been developed. Upon the analysis results, the relation for optimal combinations in terms of efficiency and degradation is proposed and the confronted trade-offs are discussed.

17/02217 Impact of gas products around the anode on the performance of a direct carbon fuel cell using a carbon/carbonate slurry

Watanabe, H. *et al. Journal of Power Sources*, 2016, 329, 567–573.

This paper investigates the impact of gas products around the anode on cell performance via an *in situ* observation. In a direct carbon fuel cell used this study, the anode is inserted into the carbon/carbonate slurry. The current–voltage (*I–V*) curves are measured before and after a long discharge in the constant current discharge mode. An *in situ* observation shows that the anode is almost completely covered by gas bubbles when the voltage becomes nearly 0 V in the constant current discharge at 40 mA/cm^2; this indicates that gas products such as CO_2 prevent the carbon particles and ions from reaching the anode. Meanwhile, the long discharge at 20 mA/cm^2 is achieved for 30 min, even though the anode is covered by the CO_2 bubbles at 15 min. The *I–V* curves at 1 min after the termination of the long discharge at 20 mA/cm^2 are lower than those prior to the long discharge. The overpotential significantly increases at higher current densities, where mass transport becomes the limiting process. The cell performance is significantly influenced by the gas products around the anode.

17/02218 Investigation of heating and cooling in a stand-alone high temperature PEM fuel cell system

Zhang, C. *et al. Energy Conversion and Management*, 2016, 129, 36–42.

One key issue pertaining to the cold-start of a high-temperature proton exchange membrane fuel cell (HT-PEMFC) is the requirement of high amount of thermal energy for heating up the stack to a temperature of 120 °C or above before it can generate electricity. Furthermore, cooling down the stack to a certain temperature (e.g. 50 °C) is necessary before stopping. In this study, the dynamic behaviour, power and energy demand of a 6 kW liquid cooled HT-PEMFC stack during heating-up, operation and cooling-down were investigated experimentally. The dynamic behaviour of fuel cell under heating-up and cooling-down processes are the mainly interested topics. Then a hybridization of HT-PEMFC with Li-ion battery to demonstrate the synergistic effect on dynamic behaviour was conducted and validated for its feasibility. At last, the concept of combining different heating sources together is analysed to reduce the heating time of the HT-PEMFC as well.

17/02219 Microbial community structure of different electrode materials in constructed wetland incorporating microbial fuel cell

Wang, J. *et al. Bioresource Technology*, 2016, 221, 697–702.

The microbial fuel cell coupled with constructed wetland (CW-MFC) microcosms were operated under fed-batch mode for evaluating the effect of electrode materials on bioelectricity generation and microbial community composition. Experimental results indicated that the bioenergy output in CW-MFC increased with the substrate concentration; maximum average voltage (177 mV) was observed in CW-MFC with carbon fibre felt (CFF). In addition, the four different materials resulted in the formation of significantly different microbial community distribution around the anode electrode. The relative abundance of *Proteobacteria* in CFF and foamed nickel (FN) was significantly higher than that in stainless steel mesh (SSM) and graphite rod (GR) samples. Notably, the findings indicate that CW-MFC utilizing FN anode electrode could apparently improve relative abundance of *Dechloromonas*, which has been regarded as a denitrifying and phosphate accumulating microorganism.

17/02220 Modeling and validation of single-chamber microbial fuel cell cathode biofilm growth and response to oxidant gas composition

Ou, S. *et al. Journal of Power Sources*, 2016, 328, 385–396.

This work describes experiments and computational simulations to analyse single-chamber, air-cathode microbial fuel cell (MFC) performance and cathodic limitations in terms of current generation, power output, mass transport, biomass competition, and biofilm growth. Steady-state and transient cathode models were developed and experimentally validated. Two cathode gas mixtures were used to explore oxygen transport in the cathode: the MFCs exposed to a helium-oxygen mixture (heliox) produced higher current and power output than the group of MFCs exposed to air or a nitrogen-oxygen mixture (nitrox), indicating a dependence on gas-phase transport in the cathode. Multi-substance transport, biological reactions, and electrochemical reactions in a multi-layer and multi-biomass cathode biofilm were also simulated in a transient model. The transient model described biofilm growth over 15 days while providing insight into mass transport and cathodic dissolved species concentration profiles during biofilm growth. Simulation results predict that the dissolved oxygen content and diffusion in the cathode are key parameters affecting the power output of the air-cathode MFC system, with greater oxygen content in the cathode resulting in increased power output and fully-matured biomass.

17/02221 Nafion-porous cerium oxide nanotubes composite membrane for polymer electrolyte fuel cells operated under dry conditions

Ketpang, K. *et al. Journal of Power Sources*, 2016, 329, 441–449.

A composite membrane operated in polymer electrolyte fuel cells (PEFCs) under low relative humidity (RH) is developed by incorporating cerium oxide nanotubes (CeNT) into a perfluorosulfonic acid (Nafion) membrane. Porous CeNT is synthesized by direct heating a precursor impregnated polymer fibres at 500 °C under an air atmosphere. Compared to recast Nafion and commercial Nafion (NRE-212) membranes, the Nafion-CeNT composite membrane generates 1.1 times higher power density at 0.6 V, operated at 80 °C under 100% RH. Compared to Nafion-cerium oxide nanoparticles (Nafion-CeNP) membrane, the Nafion-CeNT provides 1.2 and 1.7 times higher PEFC performance at 0.6 V when operated at 80 °C under 100% and 18% RH, respectively. Additionally, the Nafion-CeNT composite membrane exhibits a good fuel cell operation under 18% RH at 80 °C. Specifically, the fluoride emission rate of Nafion-CeNT composite membrane is 20 times lower than that of the commercial NRE-212 membrane when operated under 18% RH at 80 °C for 96 h. The outstanding PEFC performance and durability operated under dry conditions is mainly attributed to the facile water diffusion capability as well as the effective hydroxyl radical scavenging property of the CeNT filler, resulting in significantly mitigating both the ohmic resistance and Nafion membrane degradation.

17/02222 Nitrate removal and bioenergy production in constructed wetland coupled with microbial fuel cell: establishment of electrochemically active bacteria community on anode

Wang, J. *et al. Bioresource Technology*, 2016, 221, 358–365.

The constructed wetland coupled with microbial fuel cell (CW-MFC) systems operated at different substrate concentration and pH influents were evaluated for bioelectricity generation, contaminant removal and microbial community structure. Performance of CW-MFC was evaluated at organic loading rate of 75.3 g$COD\,m^{-3}\,d^{-1}$ and pH gradients of (5.18 ± 0.14, 7.31 ± 0.13, and 8.75 ± 0.12) using carbon fibre felt as electrodes. Peak power density was observed at slightly neutral influent condition. Compared with the open circuit CW-MFC, average chemical oxygen demand and NO_3-N removal efficiency in CW-MFC increased by 8.3% and 40.2%, respectively, under slightly neutral pH of influents. However, the removal efficiency and bioenergy production have been inhibited with acidic influents. The relative abundance of beta-*Proteobacteria*, nitrobacteria and denitrifying bacteria was significantly promoted in closed-circuit CW-MFC. Using of CW-MFC as a biochemical method for nitrate removal and bioelectricity generation under slightly neutral and alkaline influent conditions was a promising technology.

17/02223 Organic content influences sediment microbial fuel cell performance and community structure

Zhao, Q. *et al. Bioresource Technology*, 2016, 220, 549–556.

This study constructed sediment microbial fuel cells (SMFCs) with different organic loadings without the amendment of external substrates, and it investigated how such variation affects electricity generation and microbial community structure. Results found sediment characteristics significantly influenced SMFC performance and appropriate organic content is important to maintain stable power outputs. SMFCs with loss of ignition (LOI) of 5% showed the most reliable performance in this study, while high organic content (LOI 10–16%) led to higher but very unstable voltage output because of biogas accumulation and worm activities. SMFCs with low organic content (1–3%) showed low power output. Different bacterial communities were found in SMFCs shown various power generation performance even those with similar organic contents. *Thermodesulfovibrionaceae* was found closely related to the system startup and *Desulfobulbaceae* showed great abundance in SMFCs with high power production.

17/02224 PEM fuel cell model and simulation in Matlab–Simulink based on physical parameters

Abdin, Z. *et al. Energy*, 2016, 116, 1131–1144.

An advanced proton exchange membrane (PEM) fuel cell mathematical model is described and realized in four ancillaries in the Matlab–Simulink environment. Where possible, the model is based on parameters with direct physical meaning, with the aim of going beyond empirically describing the characteristics of the fuel cell. The model can therefore be used to predict enhanced performance owing to, for instance, improved electrode materials, and to relate changes in the measured performance to internal changes affecting influential physical parameters. Some simplifying assumptions make the model fairly light in computational demand and therefore amenable to extension to simulate an entire fuel-cell stack as part of an energy system. Despite these assumptions, the model emulates experimental data well, especially at high current density. The influences of pressure, temperature, humidification and reactant partial pressure on cell performance are explored. The dominating effect of membrane hydration is clearly revealed.

17/02225 Performance study of passive and active direct borohydride fuel cell employing a commercial Pd decorated Ni–Co/C anode catalyst

Zhiani, M. and Mohammadi, I. *Fuel*, 2016, 166, 517–525.

In this study, a new Pd decorated Ni–Co/C anode catalyst with remarkably high performance was introduced for using in direct borohydride fuel cell (DBFC) and compared to conventional 10 wt% Pt/C anode catalyst. The activity and poisoning tolerance of both catalysts were investigated by electrochemical techniques in half-cell. The results indicated that the Pd decorated Ni–Co/C had higher activity compared to the 10 wt% Pt/C in borohydride oxidation reaction (BOR). However, its poisoning tolerance was lower than 10 wt% Pt/C during 200 cycles. Passive DBFC results demonstrated that the cell performance and open circuit voltage (OCV) were improved by using the Pd decorated Ni–Co/C as an anode catalyst compared to commercial 10 wt% Pt/C; 126 vs 76 mW cm^{-2} and 1010 vs 892 mV, respectively. Moreover, the maximum peak power density of 761 mW cm^{-2} was obtained by Pd decorated Ni–Co/C anode catalyst in active DBFC which is comparable to generated power by H_2/O_2 proton exchange membrane fuel cell (PEMFC); 772 mW cm^{-2} at the same conditions.

17/02226 Poly iron sulfate flocculant as an effective additive for improving the performance of microbial fuel cells
Miyahara, M. *et al. Bioresource Technology*, 2016, 221, 331–335.
Laboratory microbial fuel cells were supplied with clafícial wastewater and used to examine how supplementation with poly iron sulfate, an inorganic polymer flocculant widely used in wastewater-treatment plants, affects electricity generation and anode microbiomes. It is shown that poly iron sulfate substantially increases electric outputs from microbial fuel cells. Microbiological analyses show that iron and sulfate separately affect anode microbiomes, and the increase in power output is associated with the increases in bacteria affiliated with the families *Geobacteraceae* and/or *Desulfuromonadaceae*. It is suggested that poly iron sulfate is an effective additive for increasing the electric output from microbial fuel cells. Other utilities of poly iron sulfate in microbial fuel cells are also discussed.

17/02227 Potential of porous Co_3O_4 nanorods as cathode catalyst for oxygen reduction reaction in microbial fuel cells
Kumar, R. *et al. Bioresource Technology*, 2016, 220, 537–542.
This study aims to investigate the potential of porous Co_3O_4 nanorods as the cathode catalyst for oxygen reduction reaction (ORR) in aqueous air cathode microbial fuel cells (MFCs). The porous Co_3O_4 nanorods were synthesized by a facile and cost-effective hydrothermal method. Three different concentrations (0.5, 1 and 2 mg/cm^2) of Co_3O_4 nanorods coated on graphite electrodes were used to test its performance in MFCs. The results showed that the addition of porous Co_3O_4 nanorods enhanced the electrocatalytic activity and ORR kinetics significantly and the overall resistance of the system was greatly reduced. Moreover, the MFC with a higher concentration of the catalyst achieved a maximum power density of 503 ± 16 mW/m^2, which was approximately five times higher than the bare graphite electrode. The improved catalytic activity of the cathodes could be due to the porous properties of Co_3O_4 nanorods that provided the higher number of active sites for oxygen.

17/02228 Recent progress in alkaline direct ethylene glycol fuel cells for sustainable energy production
An, L. and Chen, R. *Journal of Power Sources*, 2016, 329, 484–501.
Alkaline direct ethylene glycol fuel cells are one of the most promising power sources for portable, mobile and stationary power applications, primarily because this type of fuel cell runs on a sustainable fuel and the key materials that constitute the fuel cell are relatively inexpensive. This review article summarizes and discusses the past investigations on the development of alkaline direct ethylene glycol fuel cells, including the physical and chemical processes through the fuel cell structure, the electrocatalytic oxidation and electrocatalysts of ethylene glycol, the singe-cell performance, and innovative system designs.

17/02229 Removable air-cathode to overcome cathode biofouling in microbial fuel cells
Oliot, M. *et al. Bioresource Technology*, 2016, 221, 691–696.
An innovative microbial fuel cell (MFC) design is described, which allows the air-cathode to be replaced easily without draining the electrolyte. MFCs equipped with 9-cm^2 or 50-cm^2 bioanodes provided 0.6 and 0.7 W/m^2 (referred to the cathode surface area) and were boosted to 1.25 and 1.96 W/m^2, respectively, when the initial air-cathode was replaced by a new one. These results validate the practical interest of removable air-cathodes and evidence the importance of the cathode biofouling that takes place during the MFC starting phase. As this biofouling is compensated by the concomitant improvement of the bioanodes it cannot be detected on the power curves and may be a widespread cause of performance underestimation.

17/02230 Selection of optimal sensors for predicting performance of polymer electrolyte membrane fuel cell
Mao, L. and Jackson, L. *Journal of Power Sources*, 2016, 328, 151–160.
In this paper, sensor selection algorithms are investigated based on a sensitivity analysis, and the capability of optimal sensors in predicting polymer electrolyte membrane (PEM) fuel cell performance is also studied using test data. The fuel cell model is developed for generating the sensitivity matrix relating sensor measurements and fuel cell health parameters. From the sensitivity matrix, two sensor selection approaches, including the largest gap method, and exhaustive brute force searching technique, are applied to find the optimal sensors providing reliable predictions. Based on the results, a sensor selection approach considering both sensor sensitivity and noise resistance is proposed to find the optimal sensor set with minimum size. Furthermore, the performance of the optimal sensor set is studied to predict fuel cell performance using test data from a PEM fuel cell system. Results demonstrate that with optimal sensors, the performance of PEM fuel cell can be predicted with good quality.

17/02231 Telescopic projective Adams multiscale modeling of electrochemical reactions in tubular solid oxide fuel cells
Yang, C. *et al. Computers & Chemical Engineering*, 2016, 93, 331–342.
In order to predict the electrochemical performance of solid oxide fuel cells (SOFCs), a telescopic projective Adams (TPA) multiscale simulation method is proposed in this work. This method is constructed on the basis of the equation-free method (EFM). A lattice Boltzmann model is used as the fine-scale simulator of the proposed method. The electrochemical reaction-diffusion process was simulated by the TPA and the lattice Boltzmann method (LBM). The results of the two methods were found to be in good agreement, and the TPA method can give accurate results with lower computational costs. The electrochemical reactions were also simulated based on the TPA method. The results were consistent with the experimental data, indicating that the proposed TPA method is an effective tool to simulate the electrochemical reactions of SOFCs. Also, the proposed method is suggested to be helpful in multiscale modelling of other energy systems.

17/02232 TiO_2 inserted carbon materials with fine-tuned pore structure as effective model supports for electrocatalysts of fuel cells
Lv, Q. *et al. Carbon*, 2016, 98, 126–137.
Commercially available carbon black is a widely applied support material for nanocatalysts but notorious for its microporous structure, which is deleterious for catalysts utilization in the fuel cell application and causes numerable problems in other application areas. The development of mesoporous carbon as a substitute was proved successful but not scalable due to their intrinsic complex synthesis. In this work, a new perspective is demonstrated to circumvent the problem through blocking the micropores of carbon black by the in-situ formed TiO_2 nano/sub-nano particles. A decompression absorption method was developed where tetrabutyl titanate was pressurized into carbon pores with diameter <3 nm, succeeded by hydrolysis and calcination to form the TiO_2 inserted commercial carbon black, such as BP2000 and Vulcan XC-72. The TiO_2–C hybrid material with reduced micropore volume was found an excellent support for noble catalysts, such as Pt and Pd nanoparticles, where their insertion into carbon micropores during synthesis were prevented, thus leading to improved metal utilization. The TiO_2–C supported catalysts exhibited much superior activity and stability for methanol or formic acid electrooxidation in comparison to the plain carbon black. This work also demonstrated the negative effects of micropores in carbon support.

15 ENVIRONMENT

Pollution, health protection, applications

17/02233 Bridging the gap between energy and the environment
Holland, R. A. *et al. Energy Policy*, 2016, 92, 181–189.
To identify the most sustainable energy pathways to meet world energy demand, analyses of energy systems on which policy is based must move beyond the current primary focus on carbon to include a broad range of ecosystem services on which human well-being depends. Incorporation of a broad set of ecosystem services into the design of energy policy will differentiate between energy technology options in order to identify policies that reconcile national and international obligations to address climate change and the loss of biodiversity and ecosystem services. This paper considers the current implications of energy systems for ecosystem services and identifies key elements of an assessment. This analysis must consider the full life cycle of energy systems, the territorial and international footprint, use a consistent ecosystem service framework that incorporates the value of both market and non-market goods, and consider the spatial and temporal dynamics of both the energy and environmental system. While significant methodological challenges exist, the approach detailed can provide the holistic view of energy and ecosystem services interactions required to inform the future of global energy policy.

17/02234 Bridging the gap between sustainable technology adoption and protecting natural resources: predicting intentions to adopt energy management technologies in California

Chen, B. and Sintov, N. *Energy Research & Social Science*, 2016, 22, 210–223.

To achieve energy savings, emerging energy management technologies and programmes require customer adoption. Although a variety of models can be used to explain the adoption of energy management technologies and programs, they overlook the seemingly unconventional element of level of affiliation with nature. In fact, connectedness to nature has been identified as an important driver of many pro-environmental behaviours, but its role in pro-environmental technology adoption is also not well understood. Can affiliation with nature help to bridge the apparent gap – and complex chain of events – between sustainable technology adoption and protecting natural resources? Based on survey data from 856 southern California residents, this study investigated the influence of connectedness to nature and other factors on intentions to adopt five energy management technologies and programmes: using three platforms to monitor home energy use (website, mobile phone application, in-home display); signing up for a time-of-use pricing plan; and participating in demand response events. Regression results showed that nature connectedness was the strongest predictor of all outcomes such that higher nature connectedness predicted greater likelihood of technology and program adoption. These findings suggest that connectedness to nature may facilitate 'bridging the logic gap' between sustainable innovation adoption and environmental protection.

17/02235 Carbon balance for wood production from sustainably managed forests

Hektor, B. *et al. Biomass and Bioenergy*, 2016, 93, 1–5.

This paper approaches the CO_2 emissions from forest biomass produced in sustainable managed forests from aspects related to photosynthesis and variations in vitality and capability of CO_2 uptake, depending on, for example, different rotation periods and management regimes. These aspects are ignored or diminished in most other analyses on the subject as those analyses typically are based on simplified rigidly structured models. This paper suggests application of more relevant methodologies closer to actual real conditions. Two CO_2 issues are covered; the CO_2 balance between growth and harvesting of biomass in sustainably managed forests, and combustion of woody biomass in comparison with fossil fuels with regard to CO_2 emissions. The analysis of the first issue leads to the conclusion that biomass harvested from sustainably managed forests should be regarded as 'carbon neutral' as the vitality and CO_2 absorption is sustained and kept on the same (or better) level. Moreover, to transform old pristine forests to young vigorous forests would be an effective (long term) means of reducing atmospheric CO_2. Regarding the second issue, it was noticed that some other authors of papers on bioenergy claim that biomass would not be 'climate neutral' when used for energy as, for generation of a given energy amount, more fixed carbon is released from biomass than from fossil fuels. It is suggested here that the authors of these papers apply obsolete, too general or sometimes illogical default values. This paper suggests that emissions from the combustion of forest biomass should be compared with emissions from coal as it is the most common and relevant fuel to replace. Also additional emissions from mining/harvesting, transport, leakage, etc. should be included both for biomass and for reference fuels like coal, gas, and oil. The comparison should also be based on state-of-the-art technology, which for biomass would mean flue-gas condensing and efficient fuel treatment, for example. Under these conditions, typical biomass applications for energy would be both carbon neutral and climate neutral.

17/02236 Changes in future air quality, deposition, and aerosol-cloud interactions under future climate and emission scenarios

Glotfelty, T. *et al. Atmospheric Environment*, 2016, 139, 176–191.

The prospect of global climate change will have wide scale impacts, such as ecological stress and human health hazards. One aspect of concern is future changes in air quality that will result from changes in both meteorological forcing and air pollutant emissions. In this study, the GU-WRF/Chem model is employed to simulate the impact of changing climate and emissions following the IPCC AR4 SRES A1B scenario. An average of four future years (2020, 2030, 2040 and 2050) is compared against an average of two current years (2001 and 2010). Under this scenario, by the mid-twenty-first century global air quality is projected to degrade with a global average increase of 2.5 ppb in the maximum 8-h O_3 level and of $0.3\,\mu g\,m^{-3}$ in 24-h average $PM_{2.5}$. However, $PM_{2.5}$ changes are more regional due to regional variations in primary aerosol emissions and emissions of gaseous precursor for secondary $PM_{2.5}$. Increasing NO_x emissions in this scenario combines with a wetter climate elevating levels of OH, HO_2, H_2O_2 and the nitrate radical and increasing the atmosphere's near surface oxidation state. This differs from findings under the RCP scenarios that experience declines in OH from reduced NO_x emissions, stratospheric recovery of O_3, and increases in CH_4 and VOCs. Increasing NO_x and O_3 levels enhances the nitrogen and O_3 deposition, indicating potentially enhanced crop damage and ecosystem stress under this scenario. The enhanced global aerosol level results in enhancements in aerosol optical depth, cloud droplet number concentration, and cloud optical thickness. This leads to dimming at the Earth's surface with a global average reduction in shortwave radiation of $1.2\,W\,m^{-2}$. This enhanced dimming leads to a more moderate warming trend and different trends in radiation than those found in NCAR's CCSM simulation, which does not include the advanced chemistry and aerosol treatment of GU-WRF/Chem and cannot simulate the impacts of changing climate and emissions with the same level of detailed treatments. This study indicates that effective climate mitigation and emission control strategies are needed to prevent future health impact and ecosystem stress. Further, studies that are used to develop these strategies should use fully coupled models with sophisticated chemical and aerosol-interaction treatments that can provide a more realistic representation of the atmosphere.

17/02237 Clusters and exemplars of buildings towards zero carbon

Pan, W. and Li, K. *Building and Environment*, 2016, 104, 92–101.

In addressing anthropogenic climate change, many buildings worldwide have been designed and constructed towards zero carbon. However, their cross-context learning is largely constrained. The aim of this paper is thus to achieve a better understanding of the clusters and the energy strategy and performance of buildings towards zero carbon worldwide. The research was carried out through the combination of a two-step cluster analysis of several hundreds of low or zero carbon buildings and case studies of five exemplars. Five clusters of these buildings were revealed, which identified the gaps in the knowledge of high-rise buildings towards zero carbon and of decarbonizing the building stock. The results of the case studies of exemplars illustrate the systems integration of strategies for buildings' energy efficiency and energy generation and supply, but also indicate different concepts and calculating methodologies of 'zero carbon' or 'zero energy'. This inconsistency significantly hampers the benchmarking of buildings' energy performance and carbon reduction practices. Net-zero carbon, particularly net-zero energy, was found to be technically difficult to achieve over the one-year period of operation. The findings cast a shadow over the feasibility of achieving net zero carbon particularly for high-rise buildings due to geographic constraints for use of renewable energies, which encourages the exploration of emerging energy and carbon reduction technologies.

17/02238 Cob, a vernacular earth construction process in the context of modern sustainable building

Hamard, E. *et al. Building and Environment*, 2016, 106, 103–119.

The aim of reducing the environmental and social impacts of the building industry has led to a renewed interest in earth construction. Most of earth construction literature dealt with rammed earth or adobe techniques, but very little with cob. Yet, cob participates in the diversity of vernacular earth construction processes that value local materials and is an alternative to rammed earth and adobe in specific geographical conditions. Conservation of cob heritage also requires a better knowledge of this vernacular construction process. This bibliographical analysis gathered extensive data on cob process and summarized the different cob process variations, attempting to take into account their diversity. This analysis allowed us to provide novel data on cob process, and more specifically, (1) a clear definition of cob with regard to other earth construction processes, (2) a first summarized description of cob process that clearly distinguished its variations, (3) a list of fibres traditionally employed, (4) values and, if possible, average and standard deviation for fibre length, fibre content, manufacture water content, drying times, lift heights and wall thicknesses, (5) a summary of the strategies to manage shrinkage cracks, (6) a criterion on the quality of implementation and/or earth for cob, based on slenderness ration of lifts and (7) a discussion on the evolution of cob process with regard to societal evolutions.

17/02239 Comparative socio-cultural analysis of risk perception of carbon capture and storage in the European Union

Karimi, F. *et al. Energy Research & Social Science*, 2016, 21, 114–122.

The transition to a sustainable energy regime is not just an engineering question, but a social and cultural issue as well. This paper considers one contested technology still in development, carbon capture and storage (CCS), from a socio-cultural perspective. CCS is widely deemed to be a necessary bridging technology to a low-carbon economy, but the technology needs to pass considerable hurdles before widespread use. The importance of cultural issues in CCS deployment has been acknowledged, but research on the large-scale cultural patterns is lacking. To fill this knowledge gap, the authors combine

aggregated individual level measurements of technology opinions with indicators that characterize national cultures. The authors use survey data from a Eurobarometer together with prior cross-cultural data to show that nation-specific cultural issues can be used as a macro-level approximation of public reactions to CCS technology. Public reactions incorporate cultural factors such as the degree of separation between groups, strength of institutions over space, time and social roles, and society's tolerance for uncertainty and ambiguity. On the basis of the analysis, the authors provide a richer frame for analysts wishing to understand why and how societies and societal actors challenge and contest technologies and energy regimes.

17/02240 Development of thermal discernment among visitors: results from a field study in the Hermitage Amsterdam

Mishra, A. K. *et al. Building and Environment*, 2016, 105, 40–49.
Building energy and occupant health concerns have increased the desire for variable, dynamic indoors and hence the interest in comfort of non-uniform and/or transient thermal conditions. An extended thermal comfort field study in the Hermitage Amsterdam museum afforded a unique opportunity to analyse evolving subjective perception of occupants, upon their moving indoors, over the time they spent in the museum. Visitors' responses were grouped depending on how long they had been inside when they filled up the survey. The mean thermal sensation vote of each time group bore a strong correlation with their average time duration. For visitors who had been inside for 20 min or less, the thermal sensation vote had a significant relation with the outdoor temperature but not the indoor temperature. As visitors spent longer indoors, percentage of them feeling warm decreased and percentage of neutral or cool feeling increased. In tandem, the percentage of visitors preferring to be warmer also increased with time. Gender based differences in thermal sensation and preference also had a gradual and logical evolution with time. In an evidence of alliesthesial response, all the visitors inside for 20 min or less, accepted their thermal environment. The overall evidence suggests that visitor's subjective perception of the thermal environment undergoes a distinct evolution during their first hour indoors.

17/02241 Energy, environmental and economic impact of mini-sized and zero-emission vehicle diffusion on a light-duty vehicle fleet

Palencia, J. C. G. *et al. Applied Energy*, 2016, 181, 96–109.
Diffusion of battery electric vehicles and fuel cell hybrid electric vehicles can contribute to reduce passenger light-duty vehicle fleet CO_2 emissions. However, barriers such as higher vehicle capital cost and lack of electricity and hydrogen infrastructure prevent their deployment. A vehicle stock turnover model was used to assess the impact of mini-sized and zero-emission vehicle diffusion on passenger light-duty vehicle fleet energy and material consumption, CO_2 emissions and cost, focusing on Japan. The 2050 passenger light-duty vehicle fleet energy consumption and tank-to-wheel CO_2 emissions in the base scenario are 48.7% and 51.9% lower than the 2012 values. Diffusion of mini-sized and battery electric vehicles provides the largest energy consumption and CO_2 emissions reductions of 64.7% and 87.8% compared with the 2050 baseline values. Incremental cost of zero-emission vehicles is reduced through downsizing. The 2050 net cash flow for battery electric vehicle diffusion is reduced from 15.9 to −16.7 billion US$/year if downsizing is applied; while in the case of fuel cell hybrid electric vehicle diffusion, downsizing reduces the 2050 net cash flow from −12.5 to −47.8 billion US$/year. Thus, shifting to mini-sized zero-emission vehicles provides the quadruple benefit of reducing energy and material consumption, CO_2 emissions and cost.

17/02242 Environmental footprint assessment of building structures: a comparative study

Sinha, R. *et al. Building and Environment*, 2016, 104, 162–171.
Following the failure to implement a rather sophisticated Excel-based environmental assessment tool, environmental load profile (ELP) in the Swedish construction industry, the city of Stockholm further developed a simplified version focusing on materials to make the tool user friendly and simple, aiming at educating stakeholders in the design phase of building construction. This study evaluated whether this simplified ELP of building structures (ELP-s) can be used directly or modified for use as a simple standard model for calculating the environmental footprint of building structures. ELP-s was compared with the two leading commercial LCA softwares, GaBi and SimaPro, based on two reference buildings: (i) a concrete and (ii) a wooden building, in order to examine the importance of material selection and the simplification of the tool. The results showed that the estimated energy footprint obtained using ELP-s was close in value to that produced by GaBi and SimaPro, but that carbon footprint was much lower with ELP-s. This great deviation in carbon footprint can be explained by the lower greenhouse gas emissions intensity per unit energy in Sweden compared with the world average or European average, the major data sources on which estimations in GaBi and SimaPro are based. These results indicate the importance of exercising care when applying commercial software tools to a specific situation in a specific country. They also indicate that the model should fit the purpose.

17/02243 Environmental perceptions and health before and after relocation to a green building

MacNaughton, P. *et al. Building and Environment*, 2016, 104, 138–144.
Green buildings are designed to have low environmental impacts and improved occupant health and well-being. Improvements to the built environment including ventilation, lighting, and materials have resulted in improved indoor environmental quality (IEQ) in green buildings, but the evidence around occupant health is currently centred around environmental perceptions and self-reported health. To investigate the objective impact of green buildings on health, the authors tracked IEQ, self-reported health, and heart rate in 30 participants from green and conventional buildings for two weeks. 24 participants were then selected to be relocated to the Syracuse Center of Excellence, a LEED platinum building, for six workdays. While they were there, ventilation, CO_2, and volatile organic compound (VOC) levels were changed on different days to match the IEQ of conventional, green, and green+ (green with increased ventilation) buildings. Participants reported improved air quality, odours, thermal comfort, ergonomics, noise and lighting and fewer health symptoms in green buildings prior to relocation. After relocation, participants consistently reported fewer symptoms during the green building conditions compared to the conventional one, yet symptom counts were more closely associated with environmental perceptions than with measured IEQ. On average, participants had 4.7 times the odds of reporting a lack of air movement, 43% more symptoms (p-value = 0.019) and a 2 bpm higher heart rate (p-value < 0.001) for a 1000 ppm increase in indoor CO_2 concentration. These findings suggest that occupant health in green and conventional buildings is driven by both environmental perceptions and physiological pathways.

17/02244 Going green? The relative importance of feelings over calculation in driving environmental intent in the Netherlands and the United States

Taufik, D. *et al. Energy Research & Social Science*, 2016, 22, 52–62.
Contemporary environmental campaigns often communicate the benefits of acting environmentally friendly, assuming that larger benefits will translate into stronger intentions to act environmentally friendly – a mechanism known as 'valuation by calculation'. As such, these campaigns have neglected the possibility that decisions to act environmentally friendly can also be preceded by 'valuation by feeling', where anticipated positive feelings drive people's intention to act environmentally friendly. Acting environmentally friendly can be driven by anticipated positive feelings because it can be intrinsically rewarding to contribute to the good cause. Indeed, across two studies it was found that the stronger people anticipated to feel good about acting environmentally friendly, the stronger their intention was to act environmentally friendly. Importantly, anticipated positive feelings were a much stronger predictor of people's intention to act environmentally friendly compared to the perceived quantity of the benefits of pro-environmental actions. This indicates that environmental campaigns that resonate with people' feelings, instead of exclusively appealing to their calculations, may be an important unexploited route to encourage pro-environmental behaviour.

17/02245 High-resolution historical emission inventories of crop residue burning in fields in China for the period 1990–2013

Li, J. *et al. Atmospheric Environment*, 2016, 138, 152–161.
High-resolution historical emission inventories of crop residue burning in fields in China were developed for the period 1990–2013. More accurate time-varying statistical data and locally observed emission factors were utilized to estimate crop residue open burning emissions at provincial level. Then pollutants emissions were allocated to a high spatial resolution of 10 km × 10 km and a high temporal resolution of 1 day based on the moderate resolution imaging spectroradiometer (MODIS) fire product (MOD/MYD14A1). Results show that China's CO emissions have increased by 5.67 times at an annual average rate of 24% from 1.06 Tg in 1990 to 7.06 Tg in 2013; the emissions of CO_2, CH_4, NMVOCs, N_2O, NOx, NH_3, SO_2, $PM_{2.5}$, OC, and BC have increased by 595%, 500%, 608%, 584%, 600%, 600%, 543%, 571%, 775% and 500%, respectively, over the past 24 years. Spatially, the regions with high emissions had been notable expanding over the years, especially in the central eastern districts, the north-east of China, and the Sichuan Basin. Strong temporal pattern were observed with the highest emissions in June, followed by March to May and October. This work provides a better understanding of the spatiotemporal representation of agricultural fire emissions in China and can benefit both air quality modelling and management with improved accuracy.

17/02246 Identifying the impacts of critical habitat designation on land cover change

Nelson, E. J. *et al. Resource and Energy Economics*, 2017, 47, 89–125.
The US Endangered Species Act (ESA) regulates what landowners, land managers, and industry can do on lands occupied by listed species. The ESA does this in part by requiring the designation of habitat within each listed species' range considered critical to their recovery. Critics have argued that critical habitat (CH) designation creates significant economic costs while contributing little to species recovery. Here the authors examine the effects of CH designation on land cover change. It was found that the rate of change from 1992 to 2011 in developed (urban and residential) and agricultural land in CH areas was not significantly different compared to similar lands without CH designation, but still subject to ESA regulations. Although CH designation on average does not affect overall rates of land cover change, CH designation did slightly modify the impact of land cover change drivers. Generally, variation in land prices played a larger role in land cover decisions within CH areas than in similar areas without CH designation. These trends suggest that developers may require a greater than typical expected return to development in CH areas to compensate for the higher risk of regulatory scrutiny. Ultimately, these results bring into question the very rationale for the CH regulation. If it is for the most part not affecting land cover choices, is CH helping species recover?.

17/02247 Impacts of natural emission sources on particle pollution levels in Europe

Liora, N. *et al. Atmospheric Environment*, 2016, 137, 171–185.
This work studies of the impact of windblown dust, sea-salt aerosol and biogenic emissions on particle pollution levels in Europe. The natural emissions model (NEMO) and the modelling system consisted of the weather research and forecasting model (WRF) and the comprehensive air quality model with extensions (CAMx) were applied in a 30 km horizontal resolution grid, which covered Europe and the adjacent areas for the year 2009. Air quality simulations were performed for different emission scenarios in order to study the contribution of each natural emission source individually and together to air quality levels in Europe. The simulations reveal that the exclusion of windblown dust emissions decreases the mean seasonal PM10 levels by more than 3.3 $\mu g/m^3$ (~20%) in the eastern Mediterranean during winter while an impact of 3 $\mu g/m^3$ was also found during summer. The results suggest that sea-salt aerosol has a significant effect on PM levels and composition. Eliminating sea-salt emissions reduces PM10 seasonal concentrations by around 10 $\mu g/m^3$ in Mediterranean Sea during summer while a decrease of up to 6 $\mu g/m^3$ is found in Atlantic Ocean during autumn. Sea-salt particles also interact with the anthropogenic component and therefore their absence in the atmosphere decreases significantly the nitrates in aerosols where shipping activities are present. The exclusion of biogenic emissions in the model runs leads to a significant reduction of secondary organic aerosols of more than 90% while an increase in PM2.5 levels in central Europe and Eastern Mediterranean is found due to their interaction with anthropogenic component.

17/02248 Indoor occupancy estimation from carbon dioxide concentration

Jiang, C. *et al. Energy and Buildings*, 2016, 131, 132–141.
This paper developed an indoor occupancy estimator with which to estimate the number of real-time indoor occupants based on the carbon dioxide (CO_2) measurement. The estimator is actually a dynamic model of the occupancy level. To identify the dynamic model, the authors propose the feature scaled extreme learning machine (FS-ELM) algorithm, which is a variation of the standard extreme learning machine (ELM) but is shown to perform better for the occupancy estimation problem. The measured CO_2 concentration suffers from serious spikes. It was found that pre-smoothing the CO_2 data can greatly improve the estimation accuracy. In real applications, however, the real-time globally smoothed CO_2 data cannot be obtained. The authors, however, provide a way to use the locally smoothed CO_2 data instead, which is available in real-time. They introduce a new criterion, i.e. x-tolerance accuracy, to assess the occupancy estimator. The proposed occupancy estimator was tested in an office room with 24 cubicles and 11 open seats. The accuracy is up to 94% with a tolerance of four occupants.

17/02249 Influence of electric charges on the washout efficiency of atmospheric aerosols by raindrops

Sow, M. and Lemaitre, P. *Annals of Nuclear Energy*, 2016, 93, 107–113.
Latest investigation completed at IRSN has revealed the substantial influence of flow morphology around the drops, in atmospheric washout of fine aerosol particles by precipitations, in complement to classical mechanisms. Moreover, several authors have claimed that rain drops during stormy rainfall carry millions of elementary electric charges which could increase by couple orders of magnitude the collection efficiency as a consequence of electrostatic forces. In non-thunderstorm clouds, model calculations indicate that the image charge effect resulting from aerosol charging can significantly affect their washout, even by uncharged raindrops. However, investigations on the influence of electric charges on aerosol washout (or collection efficiency) by simulated raindrops are very fragmented and contradictory. This paper reports the results of self-charged water drop generated by hypodermic needle over charge values comparable to those reported in the literature during stormy rainfall. The authors also controllably charged aerosol particles by corona discharge and evaluate how it affects their collection efficiency. Electric charges on drops and aerosols are precisely monitored by high-resolution electrometers. The preliminary results tend to accredit the impact of electric charges in collection efficiency.

17/02250 Internalization of human labor in embodied energy analysis: definition and application of a novel approach based on environmentally extended input-output analysis

Rocco, M. V. and Colombo, E. *Applied Energy*, 2016, 182, 590–601.
One of the most controversial topics in energy analysis consists in the internalization of the effects of human labour in the embodied energy requirements of goods and services. In this paper, the bioeconomic input–output model is proposed to address such issue: it consists in a partially closed hybrid input–output model in which the production of human labor is internalized within the economy as a new productive sector. The human labour sector absorbs a portion of the national final demand, while it produces working hours in order to sustain the national economic activities. The bioeconomic model causes a reallocation of the total energy embodied in the production of goods and services due to two overlapping effects: a change in the national production technology due to the definition of the human labour sector, and a reduction in the available final demand for the consumptions of the households. The bioeconomic and the standard input–output models are comparatively applied for the analysis of (1) the energy embodied in goods and services produced by the Italian economy in 2010 and (2) the primary energy requirements of alternative dishwashing solutions in Italy. Specific embodied energy in Italian products increases by less than 5% for mining and energy industries, by 5–15% for manufacturing industries and by 15–70% for tertiary sectors. On the other hand, the energy embodied in total production from each sector may be lower or greater (from −20% to +50%) with respect to results of the standard input–output model. Moreover, it is found that the energy embodied in dishwashing by hand and by dishwasher in Italy increases by 62% and 35%, respectively, if the bioeconomic model is adopted. Based on these results, the authors argue that human labour should methodically be included alongside the supply chain of goods and services in both embodied energy analysis and life-cycle assessment.

17/02251 Organic carbon source tracing and DIC fertilization effect in the Pearl River: insights from lipid biomarker and geochemical analysis

Yang, M. *et al. Applied Geochemistry*, 2016, 73, 132–141.
The photosynthetic conversion of dissolved inorganic carbon (DIC) into organic carbon (OC) by using aquatic phototrophs in rivers may serve as a potential carbon sink, especially in the carbonate rock areas, thereby offering a clue for finding the missing carbon sink. However, primary-produced autochthonous OC is erroneously considered as terrestrial-derived allochthonous OC. Thus, carbonate weathering-related carbon sink is underestimated if only DIC concentrations sampled at river mouths are considered, and the transformation of DIC to autochthonous OC is neglected. Therefore, distinguishing sources of autochthonous and allochthonous OC is vital in the assessment of carbon sink. In this study, source-specific biomarkers, in association with chemical compositions and phytoplankton proxies in water samples collected from the Pearl River, were analysed to determine OC sources. Results showed that biomarkers in the Pearl River were quite abundant, and the calculated average autochthonous OC was approximately 65% of the total OC, indicating intense in-river primary productivity. Moreover, phytoplankton biomass and DIC concentration were positively related, indicating the DIC fertilization effect on aquatic photosynthesis. High total suspended solid (TSS) on the water surface blocked the sunlight and then reduced phytoplankton production. However, *in situ* photosynthesis of phytoplankton could also produce autochthonous OC, even larger than the allochthonous source at sites with high DIC, and even with higher TSS concentrations. These findings comprehensively elucidated the formation of autochthonous OC based on the coupling action of rock weathering and photosynthetic activity in the riverine system, suggesting a potential direction for finding the missing carbon sink.

17/02252 Processing and sorting forest residues: cost, productivity and managerial impacts

Kizha, A. R. and Han, H.-S. *Biomass and Bioenergy*, 2016, 93, 97–106.

Feedstocks generated from processing forest residues have traditionally been considered as a low value product. The economic potential of these materials can be enhanced by emerging biomass conversion technologies, such as torrefaction, briquetting, and gasification; however, these systems require higher quality feedstock. The objective of this study was to determine the cost of processing and sorting forest residues to produce feedstock, so that the best comminution machines (i.e. chipper vs grinder) could be used to better control feedstock size distribution. The tree tops left from sawlog processing and small-diameter trees were delimbed and separated from the slash pile. Three harvest units were selected and each unit was divided into three sub-treatment units (no, moderate, and intensive sorting). Results showed that the cost of operations were higher for the sorted sub-units when compared to the non-sorted. The total cost of operation (felling to loading) for sawlogs was lowest at 40.81 $\$\,m^{-3}$ in the no-sorting treatment unit, followed by moderate (42.25 $\$\,m^{-3}$) and intensive treatment unit (44.75 $\$\,m^{-3}$). For biomass harvesting, the cost of operation (felling to delimbing and sorting) ranged from 27 to 29 $\$$ oven dry metric ton^{-1}. The most expensive operational phase was primary transportation; therefore, cost of treating the forest residues had less impact on the overall cost. The cost increase (1150 $\$\,ha^{-1}$) of sorting forest residues could offset cost savings from avoided site preparation expenses (1100 $\$\,ha^{-1}$), provided that the forest residues were utilized.

17/02253 Public views on renewable energy in the Rocky Mountain region of the United States: distinct attitudes, exposure, and other key predictors of wind energy

Olson-Hazboun, S. K. *et al. Energy Research & Social Science*, 2016, 21, 167–179.

Renewable energy is often framed by policymakers and the media as an environmental or 'green' issue motivated by global climate change and the need for greenhouse gas reductions. However, some researchers studying social responses to renewables have found that factors other than opinions about climate change may be more influential in determining support for renewables. This study analyses survey data from a study of five communities in the Rocky Mountain region of the USA experiencing wind energy development to examine the relationship between environmental beliefs, climate change opinions, and support for renewable energy. Results show that views on renewable energy comprise a distinct dimension of public views on energy, environment, and climate, suggesting that public support for renewable energy is less related to environmental beliefs than to some other factors, including beliefs about economic benefits and concerns about landscape impacts. Findings also indicate that the frequency with which individuals see nearby wind turbines are strongly related to their level of support for renewable energy, while physical proximity is not. Overall, results suggest that ceasing to frame renewable energy as an environmental issue and instead framing it in a way that invokes locally relevant social values may garner broader public support.

17/02254 Real-time monitoring of personal exposures to carbon dioxide

Gall, E. T. *et al. Building and Environment*, 2016, 104, 59–67.

Elevated indoor CO_2 levels are indicative of insufficient ventilation in occupied spaces and correlate with elevated concentrations of pollutants of indoor origin. Adverse health and well-being outcomes associated with elevated indoor CO_2 levels are based on CO_2 as a proxy, although some emerging evidence suggests CO_2 itself may impact human cognition. Using portable monitors, the authors conducted an exposure study with 16 subjects in Singapore to understand the levels, dynamics and influencing factors of personal exposure to CO_2. Participants carried a CO_2 monitor continuously for 7-day periods recording their exposure levels at 1-min intervals. A recall diary was maintained of time-microenvironment-activity budget. It was found that the mode of bedroom ventilation was a major determinant of CO_2 exposure. Approximately half of the participants slept in bedrooms employing ductless split air-conditioners (group AC); half slept in bedrooms naturally ventilated through operable windows (group NV). Median CO_2 exposure levels for AC vs NV groups are significantly different ($\bar{x}_{AC} = 650$ ppm vs $\bar{x}_{NV} = 550$ ppm, $p < 0.001$). Mean daily integrated exposures for group AC were statistically higher than for group NV: 22,800 ppm h/d vs 16,000 ppm h/d ($p < 0.005$). Exposure events associated with potential adverse cognitive implications (duration > 2.5 h, average CO_2 mixing ratio > 1000 ppm) occurred, on average, at frequencies of 0.5 d^{-1} across all participants, 0.6 d^{-1} for AC participants and 0.2 d^{-1} for NV participants. The majority of such events occurred in the home (86%), followed by work (9%) and transit (3%).

17/02255 Recovery and diversity of the forest shrub community 38 years after biomass harvesting in the northern Rocky Mountains

Jang, W. *et al. Biomass and Bioenergy*, 2016, 92, 88–97.

This study investigated the long-term impact of biomass utilization on shrub recovery, species composition, and biodiversity 38 years after harvesting at Coram experimental forest in north-western Montana, USA. Three levels of biomass removal intensity (high, medium and low) treatments combined with prescribed burning treatment were nested within three regeneration harvest treatments (shelterwood, group selection and clear-cut). Four shrub biomass surveys (pre-treatment, 2, 10 and 38 years after treatment) were conducted. Shrub biomass for all treatment units 38 years after treatment exceeded the pre-treatment level, and biomass utilization intensity did not affect shrub recovery (ratio of dry biomass at time t to pre-treatment biomass). Species composition changed immediately after harvesting (2 years); however, the species composition of treated units did not differ from the untreated control 38 years after harvesting. Biodiversity indices (Shannon's and Pielou's indices) also decreased immediately following harvesting, but recovered 10 years after harvesting. The responses of diversity indices over time differed among biomass utilization levels with the high-utilization level and unburned treatment producing the most even and diverse species assemblages 38 years after harvesting. The results indicate the shrub community is quite resilient to biomass harvesting in this forest type.

17/02256 Roadside air quality and implications for control measures: a case study of Hong Kong

Ai, Z. T. *et al. Atmospheric Environment*, 2016, 137, 6–16.

Traffic related air pollution is one of major environmental issues in densely populated urban areas including Hong Kong. A series of control measures has been implemented by Hong Kong government to cut traffic related air pollutants, including retrofitting the Euro II and Euro III buses with selective catalytic reduction (SCR) devices to lower nitrogen dioxide (NO_2) emissions. In order to reveal the real-life roadside air quality and evaluate the effectiveness of the control measures, this study first analysed the recent 6-year data regarding concentrations of pollutants typically associated with traffic recorded in two governmental roadside monitoring stations and second conducted on-site measurements of concentration of pollutants at pedestrian level near five selected roads. Given that there is a possibility of ammonia leakage as a secondary pollutant from SCR devices, a special attention was paid to the measurements of ammonia level in bus stations and along roadsides. Important influencing factors, such as traffic intensity, street configuration and season, were analysed. Control measures implemented by the government are effective to decrease the traffic emissions. In 2014, only NO_2 cannot achieve the annual air quality objective of Hong Kong. However, it is important to find that particulate matters, rather than NO_2, post potentially a short-term exposure risk to passengers and pedestrians. Based on the findings of this study, specific control measures are suggested, which are intended to further improve the roadside air quality.

17/02257 Scenario-based potential effects of carbon trading in China: an integrated approach

Zhang, C. *et al. Applied Energy*, 2016, 182, 177–190.

Using China's provincial panel data and national panel data of Organization for Economic Co-operation and Development (OECD) and five major emerging national economies: Brazil, Russia, India, China and South Africa, this paper simulates the scenario-based potential effect of carbon trading in China. Analysis methods included stochastic frontier analysis, difference-in-differences model, and non-linear programming technique. Results indicated that in a theory-based view of carbon trading, the shadow price of carbon dioxide generally rises, with a non-linear negative correlation with carbon dioxide emissions. In different regions, the shadow price of carbon dioxide presents a digressive tendency among eastern, central, and western areas, with divergent gaps between and within areas. When the greatest goal is assumed to reduce national carbon intensity as much as possible at the given national gross domestic product (GDP) (scenario I), carbon trading has the effect of reducing carbon intensity by 19.79%, with the consideration of Porter hypothesis effect. If the rigid constraint of national GDP is relaxed, and the dual constraint of both economic growth and environment protection in each region is introduced (scenario II), the resulting effect is a reduced carbon intensity of 25.24%. China's general carbon intensity in 2012 was higher than goals set at the Copenhagen Conference, but lagged behind the goal of twelfth Five-Year Plan for China's national economy. This study provides realistic and significant technical support for the government to use in designing and deploying a national carbon trading market.

17/02258 Shared and practical approach to conserve utilities in eco-industrial parks

Nair, S. K. *et al. Computers & Chemical Engineering*, 2016, 93, 221–233.

Conserving utilities in an eco-industrial park (EIP) by exploiting the synergistic heating/cooling needs of its inhabitants can have significant economic and environmental benefits. However, a successful implementation of an EIP-wide heat integration involves much more

than the simple minimization of utility usage. Like any collaborative endeavour involving independent and diverse profit-making enterprises, an EIP-wide heat integration faces several real and practical challenges such as exchanger locations, stream transports over long distances, etc. This work proposes a mixed-integer non-linear programming model for configuring an EIP-wide multi-enterprise heat exchanger network (HEN). The authors propose a practical and rational strategy that (1) considers all the major capital and operating costs, and utility savings, (2) selects an optimum HEN location with the highest net present value, (3) uses a third-party logistics provider for managing and operating the HEN, and (4) ensures an identical rate of return on investment for all participating enterprises.

17/02259 Steady-state and transient thermal measurements of green roof substrates

Pianella, A. *et al. Energy and Buildings*, 2016, 131, 123–131.

There has been growing interest in using extensive green roofs for commercial and residential buildings in urban areas. Green roofs provide many benefits, including adding an additional insulation layer. The potential of this benefit depends on many factors, including the thermal properties of the green roof substrate. Thermal conductivity values of three substrates comprised primarily of scoria, crushed roof tile and bottom-ash were measured with steady-state and transient techniques under three moisture conditions. Specific heat capacities of the green roof substrates were also measured with a transient technique. Steady-state measurements were performed with a 'k-Matic' apparatus while transient measurements with KD2 Pro needles. In general, the steady-state measurements showed more consistency than transient measurements. Thermal conductivity differed among the three substrates: crushed roof tile had the highest conductivity values across all moisture contents. Substrate moisture content consistently increased thermal conductivity across all substrates, but this was significantly greater for the crushed roof tile substrate. Steady-state thermal conductivity curves were fitted using the thermal conductivity model for green roof substrates proposed earlier. The coefficients obtained are presented and can be used in green roof models to quantify the thermal performance of green roofs and building energy savings.

17/02260 Study on the identification of main drivers affecting the performance of human operators during low power and shutdown operation

Kim, A. R. *et al. Annals of Nuclear Energy*, 2016, 92, 447–455.

In the past, many researchers believed that a reactor during low power and shutdown operation was sufficiently safe. This belief has been changed by the number of accidents during such types of operation, which is significantly high. Also, it was pointed out that one of the main differences between low power and shutdown operation and full power operation is the significance of human action because there are huge amounts of human actions due to extensive maintenance and testing while automatic control and safety functions may be disabled and procedures are insufficient or incomplete. This paper suggests the main drivers in performing human reliability analysis. This study reviewed eight reports relating to human performance during low power and shutdown operation and applied a root cause analysis method for 53 human or human-related events at domestic nuclear power plants to derive the main drivers that affect the occurrence of those events. As a result, several main drivers were derived, such as procedures, training, experience of personnel, and workload/stress. It is expected that these main drivers will be used to perform human reliability analysis for low power and shutdown operation.

17/02261 The 21st century population-energy-climate nexus

Jones, G. A. and Warner, K. J. *Energy Policy*, 2016, 93, 206–212.

The world population is projected to reach 10.9 billion by 2100, yet nearly one-fifth of the world's current 7.2 billion live without access to electricity. Though universal energy access is desirable, a significant reduction in fossil fuel usage is required before mid-century if global warming is to be limited to $<2\,^{\circ}C$. Here the authors quantify the changes in the global energy mix necessary to address population and climate change under two energy-use scenarios, finding that renewable energy production (9% in 2014) must comprise 87–94% of global energy consumption by 2100. This study suggests >50% renewable energy needs to occur by 2028 in a $<2\,^{\circ}C$ warming scenario, but not until 2054 in an unconstrained energy use scenario. Given the required rate and magnitude of this transition to renewable energy, it is unlikely that the $<2\,^{\circ}C$ goal can be met. Focus should be placed on expanding renewable energy as quickly as possible in order to limit warming to 2.5–3 $^{\circ}C$.

17/02262 The distributional effects of emissions taxation in Brazil and their implications for climate policy

da Silva Freitas, L. F. *et al. Energy Economics*, 2016, 59, 37–44.

The emission of greenhouse gases (GHG) generated by human activity is a major cause of global warming and climate change. There is considerable debate about the choice of the best mechanism to reduce emissions under a climate policy. The aim of this paper is to measure the impact of a policy of taxing GHG emissions on the Brazilian economy as a whole and on different household groups based on income levels in 2009. The following databases were used: Supply and Use Tables, Household Budget Survey, National Household Sample Survey and emissions data from the Brazilian Ministry of Science and Technology and Innovation. A price system from a national input–output model that incorporates the intensity of GHG emissions is used, as well as a consumption vector broken down into ten representative households with different income levels. The main results indicate that this taxation system was slightly regressive and had a small negative impact on output. There were, however, significant emissions reductions.

17/02263 The importance of temperature and thermoregulation for optimal human sleep

Joshi, S. S. *et al. Energy and Buildings*, 2016, 131, 153–157.

In the last few decades, there has been a decline in average sleep duration and quality that has adversely affected general health of the population. Increased use of artificial lighting, television, noise, and light-emitting gadgets in the post-industrial society has led to an environment full of factors that can adversely affect sleep. Sleep is essential for the restoration of health and well-being, and has a direct effect on the quality of life of an individual. It is thus imperative to design constructions that provide a sleep permissive environment. In addition to environmental factors, sleep and wakefulness in humans is affected by a multitude of physiological parameters as well. The mechanisms and interplay between these factors that influence sleep permissiveness or promotion have received relatively little attention. The present review takes a holistic approach in explaining the basic circadian and homeostatic processes that influence sleep and sleepiness, and then delves deeper into how the thermal rhythms of the body affect these processes. It also discusses previous research and models in construction design that influence ambient temperature, skin surface temperature, and other thermoregulatory factors that can be controlled for optimal sleep.

17/02264 The influence of personality traits on occupant behavioural patterns

Schweiker, M. *et al. Energy and Buildings*, 2016, 131, 63–75.

Occupant behaviour in office buildings and its driving forces have been investigated intensely. Despite huge individual differences, these analyses are mainly performed on aggregated levels. Attempts are scarce to explain underlying mechanisms which personal characteristics lead to observed differences. This study presents a unique analysis of the influence of personality traits on four types of behavioural patterns – clothing adjustments, window opening, blind closing, and interactions with a ceiling fan – and two dimensions of thermal perception – sensation and preference. As personality traits, three of the big five personality traits describing human personality, namely neuroticism, extraversion, and openness to new experiences, together with the concepts of general and thermo-specific self-efficacy were analysed. The data set used derived from experimental studies in a semi-controlled climate chamber with single occupied offices consisting of 65 subjects. Throughout the analysis, multivariate logistic, linear, and ordinal mixed effect model analyses were performed. According to the results, all personality traits lead to significant differences between behavioural patterns. Thermal sensation was affected significantly by extraversion, thermal preference by neuroticism, openness and thermo-specific self-efficacy. Together with additional experimental and field studies these results can form a basis for theory-driven occupant behavioural profiles used in building performance simulation.

17/02265 The psychology of participation and interest in smart energy systems: comparing the value-belief-norm theory and the value-identity-personal norm model

van der Werff, E. and Steg, L. *Energy Research & Social Science*, 2016, 22, 107–114.

Environmental problems can be reduced if people would participate in smart energy systems. Little is known about which factors motivate people to actually participate in smart energy systems. The authors tested the factors that influence individuals' interest and actual participation in smart energy systems. They compared the predictive power of the value-belief-norm theory with a novel model to explain pro-environmental actions: the value-identity-personal norm model. Both focused on normative considerations in explaining behaviour, but the VIP model focused on general rather than behaviour-specific antecedents. The results show that both models explained a similar amount of variance in interest and actual participation in smart energy systems. This suggests that the value-identity-personal norm model is a promising model to explain and promote pro-environmental actions such as participation in smart grids. Further, it is more parsimonious

than the value-belief-norm theory and focuses on general factors that are likely to predict other environmental behaviours as well. The value-identity-personal norm model is therefore a particularly promising model in promoting a range of environmental behaviours.

17/02266 Towards an understanding of the marine fouling effects on VIV of circular cylinders: response of cylinders with regular pyramidal roughness

Zeinoddini, M. *et al. Applied Ocean Research*, 2016, 59, 378–394.

The underwater surfaces of man-made structures quickly become covered by unwanted aquatic organisms. These organisms change the flow regime around the structure. Despite the important contributions of previous studies on the vortex induced vibration (VIV) of bluff bodies, the flow induced vibration of non-stationary cylinders covered by marine fouling appears not to have received due attentions in the literature. The current paper reports on an attempt for better understanding the marine fouling effects on the VIV of circular cylinders. A structured review of the literature related to the fluid structure interactions in marine fouled cylinders is first presented. Results of an experimental study on the VIV of low mass-damping circular cylinders with artificial marine fouling are then reported. The fouling was simulated by uniformly distributed pyramids on the surface of the test cylinders. The Reynolds number ranged from 3.5×10^3 to 3.5×10^4. The experimental results showed that, the peak VIV amplitude, the synchronization range, the lift force coefficient, the mean drag coefficient and the RMS of the fluctuating drag coefficient were decreased by the fouling. Flow visualization showed that the separation was delayed and the vortices size and recirculation length became shorter in the fouled cylinder. In general, it appeared that the fouling was acting, to some degrees, as a VIV suppression tool.

17/02267 Tuning graphene for energy and environmental applications: oxygen reduction reaction and greenhouse gas mitigation

Haque, E. *et al. Journal of Power Sources*, 2016, 328, 472–481.

Porous nitrogen-doped graphene samples were synthesized and tuned via pyrolysis of solid nitrogen precursor dimethyl-aminoterephthalate with graphene oxide as template. The investigations show that the extent of thermal treatment, total concentration of nitrogen and the nature of nitrogen moieties play important roles in enhancing oxygen reduction reaction (ORR) and CO_2 uptake. N-doped graphene synthesized at 650 °C (NG-650) with specific BET surface area of 278 m^2/g, exhibits enhanced CO_2 sorption capacity of 4.43 mmol/g (at 298 K, 1 bar) with exceptional selectivity ($CO_2:N_2 = 42$) and cyclic regeneration stability. In contrast, nitrogen-doped graphene synthesized at 750 °C (NG-750) demonstrated excellent catalytic activity for ORR via favourable $4e^-$ transfer, performance stability with tests conducted up to 5000 cycles, and is unaffected by methanol cross-over effect. Thus, NG-750 shows potential to replace metal-based electrodes for fuel cell application. The comparative results for ORR with non-doped and nitrogen-doped graphene electrodes showed that graphitic nitrogen sites play vital role in enhancing catalytic activity.

17/02268 Ultrafine particle size as a tracer for aircraft turbine emissions

Riley, E. A. *et al. Atmospheric Environment*, 2016, 139, 20–29.

Ultrafine particle number (UFPN) and size distributions, black carbon, and nitrogen dioxide concentrations were measured downwind of two of the busiest airports in the world, Los Angeles International Airport (LAX) and Hartsfield-Jackson International Airport (ATL – Atlanta, GA) using a mobile monitoring platform. Transects were located between 5 and 10 km from the ATL and LAX airports. In addition, measurements were taken at 43 additional urban neighbourhood locations in each city and on freeways. A three- to five-fold increase was found in UFPN concentrations in transects under the landing approach path to both airports relative to surrounding urban areas with similar ground traffic characteristics. The latter UFPN concentrations measured were distinct in size distributional properties from both freeways and across urban neighbourhoods, clearly indicating different sources. Elevated concentrations of black carbon (BC) and NO_2 were also observed on airport transects, and the corresponding pattern of elevated BC was consistent with the observed excess UFPN concentrations relative to other urban locations.

17/02269 We forgot half of the population! The significance of gender in Danish energy renovation projects

Tjørring, L. *Energy Research & Social Science*, 2016, 22, 115–124.

Energy renovations are considered to have great potential for reducing the problem of excessive energy consumption. Thus far, initiatives to increase the number of energy renovations have mostly consisted of financial incentives and technical home solutions. Such initiatives overlook the fact that the way people live their everyday lives plays a crucial role in understanding why they choose whether to perform an energy renovation. This study is based on an anthropological investigation of 10 Danish families and their decision-making process while receiving free energy advice, which, in many cases, ended as an energy renovation project in the home. During the study, gender emerged as a significant factor in two ways. First, energy renovations were perceived differently by men and women as a consequence of their different everyday practices. Second, there was a cultural norm about the division between what men and women do in the home. This cultural norm placed energy renovation in the male sphere of interest. These findings call for new methods to increase the number of energy renovations that focus on the home, not only as a technical issue that can be improved but also as a living space that contains different gender practices and cultural influences.

CO_2, NO_x, SO_2 and particulate emissions

17/02270 A geographical assessment of vegetation carbon stocks and greenhouse gas emissions on potential microalgae-based biofuel facilities in the United States

Arita, C. Q. *et al. Bioresource Technology*, 2016, 221, 270–275.

The microalgae biofuel life cycle assessments (LCA) present in the literature have excluded the effects of direct land-use change (DLUC) from facility construction under the assumption that DLUC effects are negligible. This study seeks to model the greenhouse gas (GHG) emissions of microalgae biofuels including DLUC by quantifying the CO_2 equivalence of carbon released to the atmosphere through the construction of microalgae facilities. The locations and types of biomass and soil organic carbon that are disturbed through microalgae cultivation facility construction are quantified using geographical models of microalgae productivity potential including consideration of land availability. The results of this study demonstrate that previous LCA of microalgae to biofuel processes have overestimated GHG benefits of microalgae-based biofuels production by failing to include the effect of DLUC. Previous estimations of microalgae biofuel production potential have correspondingly overestimated the volume of biofuels that can be produced in compliance with the USA's environmental goals.

17/02271 Bi-lateral CO_2 emissions embodied in Australia–China trade

Jayanthakumaran, K. and Liu, Y. *Energy Policy*, 2016, 92, 205–213.

This paper quantifies the CO_2 emissions embodied in bi-lateral trade between Australia and China using a sectoral input–output model. The results revealed: (1) that China performs lower than Australia in clean technology in the primary, manufacturing, energy sectors due to their overuse of coal and inefficient sectoral production processes, and (2) that China had a 30.94 Mt surplus of bi-lateral CO_2 emissions in 2010–2011 and (3) overall global emissions were reduced by 20.19 Mt through Australia–China trade in 2010–2011. The result indicates that the greater the energy efficient a country among the trading partners the lower will be the overall global CO_2 emissions. Global emissions decreased mainly because China consumed Australian primary products rather than producing them. Australia is an energy efficient producer of primary products relative to China. The bilateral trade compositions and trade volume played an important role in lowering global emissions and therefore one can view proposed China Australia Free trade Agreement positively in reducing global emissions. However, for the sustainable development, China should strengthen clean energy use and both countries should adopt measures to create an emission trading scheme in order to avoid protectionism in the form of future border price adjustments.

17/02272 Carbon dioxide and methane supersaturation in lakes of semi-humid/semi-arid region, northeastern China

Wen, Z. *et al. Atmospheric Environment*, 2016, 138, 65–73.

Understanding concentrations of carbon dioxide (CO_2) and methane (CH_4) in lakes is an important part of a comprehensive global carbon budget. The authors estimated data on the partial pressure of CO_2 (pCO_2) and CH_4 (pCH_4) from sampling with 95 lakes in semi-humid/semi-arid region of north-eastern China during ice-free period. Both pCO_2 and pCH_4 varied greatly among the study sites. $p(CO_2)$ values in these lakes ranged from 21.9 to 30,152.3 µatm ($n = 403$), and 91% of lakes in this survey were supersaturated with CO_2. $p(CH_4)$ values ranged from 12.6 to 139,630.7 µatm with all sites in this study of CH_4 sources to the atmosphere during the ice-free period. The collected urban lakes samples exhibited higher pCO_2 and pCH_4 than wild lakes samples. Either the mean value of $p(CO_2)$ or $p(CH_4)$ in saline waters is higher than in fresh waters. Correlation analysis implied that the partial pressure of the greenhouse gases (CO_2 and CH_4) showed

statistically correlations with water environment indicators like pH, dissolved organic carbon (DOC), total nitrogen (TN), total phosphorus (TP), and chlorophyll *a* (*Chla*). However, the most of the relationships showed a high degree of scatter, only pH might be used as the predictor of the gas partial pressure based on the result of this study ($r_{pCO2} = -0.437$, $p < 0.01$, $n = 382$; $r_{pCH4} = -0.265$, $p < 0.01$, $n = 400$). Furthermore, salinity could be a good predictor for $p(CO_2)$ and $p(CH_4)$ in 83 freshwater lakes in this study ($r_{pCO2} = 0.365$, $r_{pCH4} = 0.323$, $p < 0.01$, $n = 348$). The mean CO_2 flux increased with the decreasing lake area size. The calculated annual areal carbon emission rate is $560.2\,g\,C\,m^{-2}$ from 95 lakes in north-eastern China. It was not possible to extrapolate carbon emissions from these lakes to the boreal region or a wider scale because of the change of environmental conditions.

17/02273 Club convergence and clustering of U.S. energy-related CO_2 emissions

Burnett, J. W. *Resource and Energy Economics*, 2016, 46, 62–84.

This study examines the convergence of energy-related carbon dioxide emissions among a panel of US states between the period 1960–2010. This examination is carried out by means of a two-stage procedure. In the first stage, the authors conducted an endogenous grouping, regression-based convergence test. Unlike previous studies, this methodology endogenously identifies groups of states with emissions that are converging to a similar steady state growth path over time. In the second stage, they evaluated the conditional rate of convergence for the whole sample and for each club using panel data, fixed effects models that control for unobserved, time-invariant heterogeneous effects. More specifically, the authors examined the rates of convergence conditional on certain structural and non-structural characteristics of the state economy. Results from stage one and stage two suggest that one group of twenty-six states is converging to a unique steady-state equilibrium, and otherwise, the remaining states are diverging. Finally, different policy approaches to mitigating carbon dioxide emissions based on the club convergence hypothesis were discussed.

17/02274 Combustion characteristics and NO_X emissions of biogas fuels with various CO_2 contents in a micro co-generation spark-ignition engine

Kim, Y. *et al. Applied Energy*, 2016, 182, 539–547.

Biogas is a renewable alternative fuel for internal combustion engines that has several advantages over conventional fuels, including lower costs and reduced levels of harmful emissions. In particular, it exhibits a neutral recirculation loop for carbon dioxide (CO_2), which is one of the main causes of global warming. This study investigated biogas fuels with various compositions using a micro co-generation engine system. The ratio of methane to CO_2 and engine load were varied, and the intake air and fuel flow rates were controlled to change the equivalence ratio. The results show that for a given engine load, the ignition delay and combustion period increased with CO_2 content, and the combustion speed decreased. The fuel consumption increased slightly with CO_2 content; however, the thermal efficiency improved using a lean burn strategy, resulting in lower nitrogen oxide (NO_X) emission, and moreover, the use of biogas with the stoichiometric air–fuel ratio appears effective in reducing NO_X emissions and can improve the fuel economy at higher loads.

17/02275 Constraining the sulfur dioxide degassing flux from Turrialba volcano, Costa Rica using unmanned aerial system measurements

Xi, X. *et al. Journal of Volcanology and Geothermal Research*, 2016, 325, 110–118.

Observed sulfur dioxide (SO_2) mixing ratios on-board unmanned aerial systems (UAS) during March 11–13, 2013 are used to constrain the three-day averaged SO_2 degassing flux from Turrialba volcano within a Bayesian inverse modelling framework. A mesoscale model coupled with Lagrangian stochastic particle backward trajectories is used to quantify the source-receptor relationships at very high spatial resolutions (i.e. <1 km). The model shows better performance in reproducing the near-surface meteorological properties and observed SO_2 variations when using a first-order closure non-local planetary boundary layer (PBL) scheme. The optimized SO_2 degassing fluxes vary from 0.59 ± 0.37 to $0.83 \pm 0.33\,kt\,d^{-1}$ depending on the PBL scheme used. These fluxes are in good agreement with ground-based gas flux measurements, and correspond to corrective scale factors of 8–12 to the post-eruptive SO_2 degassing rate in the AeroCom emission inventory. The maximum a posteriori solution for the SO_2 flux is highly sensitive to the specification of prior and observational errors, and relatively insensitive to the SO_2 loss term and temporal averaging of observations. These results indicate relatively low degassing activity but sustained sulfur emissions from Turrialba volcano to the troposphere during March 2013. This study demonstrates the utility of low-cost small UAS platforms for volcanic gas composition and flux analysis.

17/02276 CO_2 capture using limestone for cultivation of the freshwater microalga *Chlorella sorokiniana* PAZ and the cyanobacterium *Arthrospira* sp. VSJ

Zawar, P. *et al. Bioresource Technology*, 2016, 221, 498–509.

The present study reports a process wherein CO_2 is captured in the form of bicarbonates using calcium oxide and photosynthetically fixed into biomass. Microalgal cultures, namely *Chlorella sorokiniana* PAZ and *Arthrospira* sp. VSJ were grown in the medium containing bicarbonates. The rate of bicarbonate utilization by *C. sorokiniana* PAZ was higher when CO_2 trapped in the presence of 2.67 mM calcium oxide than in the presence of 10 mM sodium hydroxide and with direct addition of 10 mM sodium bicarbonate. For *Arthrospira* sp. VSJ the bicarbonate utilization was 92.37%, 88.34% and 59.23% for the medium containing CaO, NaOH and $NaHCO_3$, respectively. Illumination of photosynthetically active radiation (PAR) + ultraviolet A radiation (UVA) enhanced the yield of *C. sorokiniana* PAZ and *Arthrospira* sp. VSJ by 1.3- and 1.8-fold, respectively. Fourier transform infrared analysis revealed elevation in the biosynthesis of specific metabolites in response to the UVA exposure.

17/02277 CO_2 regeneration performance enhancement by nanoabsorbents for energy conversion application

Lee, J. H. *et al. Applied Thermal Engineering*, 2016, 103, 980–988.

Due to the recent increase in the consumption of energy and the use of fossil fuels, global warming has become a serious issue. To address this problem, CO_2 gas, which is the major element of the greenhouse gases, should be captured, regenerated and converted to useful fuels. The integrated gasification combined cycle (IGCC) and cement process generate large amount of CO_2, which are controlled through pre-combustion capture. However, this method has a disadvantage because the system temperature should be decreased to $-20\,^{\circ}C$ or lower. Therefore, the development of new absorbent is required to reduce the energy consumed for refrigeration. There is a study that improved the CO_2 absorption performance by adding Al_2O_3 nanoparticles to methanol. However, studies on the regeneration of CO_2 in nanofluid absorbents (nanoabsorbents) are insufficient. Therefore, in this study, the CO_2 regeneration performance in Al_2O_3 nanoabsorbents is evaluated. It is found that the regeneration performance of CO_2 is improved by 16% by using nanoabsorbents compared to methanol. Furthermore, the CO_2 regeneration characteristics of nanoabsorbents are analysed by considering the detachment time of CO_2 bubbles from the surface, the cross-sectional area of CO_2 bubble, and the number of regeneration sites through the CO_2 regeneration and bubble visualization experiments. It is concluded that the mechanism of surface effect is the most plausible to explain the CO_2 regeneration performance enhancement by nanoabsorbents.

17/02278 Determination of effective diffusivities and convective coefficients of CO_2 in gypsum plasters by dynamic single pellet experiments

Kalender, M. *Building and Environment*, 2016, 105, 164–171.

This paper presents the effective diffusion and convective coefficients obtained for construction gypsum, perlite, and machine plaster pellets by using a dynamic single pellet moment technique at various temperature, and at different pressure drops. The experimental studies were performed by isobaric and non-isobaric conditions across between the upper and lower surfaces of the pellets. The experimental moment values obtained from the experiments carried out were used to calculate desired coefficients such as the effective diffusivity, tortuosity factor, *D* parameter, and Darcy coefficient. The experimental results for CO_2 diffusion in the pellets with porous at isobaric conditions showed that the effective diffusivity values for all gypsum plasters increase with increasing both pellet porosity and the temperature. It was observed that the tortuosity factor depends on macro porosity of the pellets used. The results indicated that the diffusion mechanism for all gypsum plasters is the transient regime diffusion. The effective diffusivity values decreased with increasing the pressure drop. In the range of pressure drop studied, both diffusive (at low pressure drops) and viscous (at high pressure drops) flows for CO_2 diffusion in construction gypsum and perlite plasters were dominant. But, the diffusion flow type which is important for machine plaster was only the viscous flow at all pressure drops. Finally, the Darcy coefficients of the gypsum plaster pellets were calculated. It was observed that the results were in agreement with the literature results obtained for porous solids similar to porous gypsum plaster pellets used in this study.

17/02279 Development of an equilibrium theory solver applied to pressure swing adsorption cycles used in carbon capture processes

Oreggioni, G. *et al. Computers & Chemical Engineering*, 2016, 94, 18–27.

An equilibrium theory simulator (Esim) for the simulation of cyclic adsorption processes is presented. The equations are solved with a Godunov upwind flux scheme that does not require either the

evaluation of characteristics or shock equations or the imposition of a numerical entropy condition to track shocks. Esim is able to simulate non-trace and non-isothermal adsorption systems with any adsorption isotherm. Esim has been validated against gPROMS based simulations that use the full set of governing equations (including mass and heat transfer resistances and axial dispersion) carried out under conditions close to the limits where equilibrium theory is valid. Esim enables the establishment of bounds for the optimal performance of an equilibrium driven separation and requires only the measurement of adsorption isotherms.

17/02280 Effect of carburization protocols on molybdenum carbide synthesis and study on its performance in CO hydrogenation

Mo, T. *et al. Catalysis Today*, 2016, 261, 101–115.

Molybdenum carbides were prepared under different carburization conditions. The role of carburization protocol was studied while their CO hydrogenating performances were evaluated in a fixed-bed reactor at 280 °C, 3.1 MPa and $H_2/CO = 2.0$. The structure of the carbides mainly depended on the type and concentration of carbon source while the crystallite size depended on carbon source and temperature. The surface area, morphology and surface carbon deposition phenomenon of the carbides were sensitive to heating rate and holding time other than the above factors. Though the bulk structure was the same at a carburization temperature range from 630 to 760 °C, the carburization degree of the carbides was changing continuously. This diversity led the bond strength of molecular adsorbed CO weaken at a higher carburization temperature while the adsorptive strength of H_2 was hardly changed. Both the adsorptive quantities of CO and H_2 followed the same trend, with the highest amount on the carbide prepared at 630 °C. The activities of the catalysts correlated well with their adsorptive quantities of CO and H_2, and the product selectivity was related to their hydrogenation capacity.

17/02281 Effects of ionic liquid dispersion in metal-organic frameworks and covalent organic frameworks on CO_2 capture: a computational study

Xue, W. *et al. Chemical Engineering Science*, 2016, 140, 1–9.

A systematic computational study was performed in this work to investigate the dispersion behaviours of ionic liquids (ILs) in metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) as well as the separation performance of the resulting composites for CO_2/CH_4 and CO_2/N_2 mixtures. Five MOFs and eight COFs with diverse pore structures and chemical properties were selected as the supporters for 1-n-butyl-3-methylimidazolium thiocyanate [BMIM][SCN]. The results show that stronger Coulombic interactions contributed from the frameworks of MOFs can lead to better dispersion of the IL molecules in their pores compared with COFs. The gas separation performance can be significantly enhanced by introducing [BMIM][SCN] into MOFs and COFs, and MOFs can be considered as better support materials for ILs. Better dispersion of the IL in a given support material will induce greater enhancement on the separation performance of the composite, and such phenomenon is more evident for CO_2/CH_4 mixture compared with the CO_2/N_2 system. The IL molecules are more inclined to aggregate in the 2D-COFs and MOFs with 1D pore structures. However, they are more dispersive in the materials with 3D pore structures as the supporters, leading to a more evident improvement on the separation performance. This work also shows that using the materials containing strong adsorption sites like coordinatively unsaturated metal sites as the supporters for ILs cannot achieve significant enhancement on the gas separation performance of the composites.

17/02282 Heat integration of alternative Ca-looping configurations for CO_2 capture

Lara, Y. *et al. Energy*, 2016, 116, 956–962.

The best option to overcome the energy penalty in Ca-looping is to take advantage of the surplus heat by external integration to produce additional power and increase net efficiency. As calciner represents the main energy consumption, another possibility is to internally use the surplus heat to preheat the solids entering this reactor. The objective of internal integration is to reduce the energy demand per captured tonne of CO_2. It represents a reduction of the coal and oxygen needs and also a total decrease in the CO_2 generation regarding the ordinary configuration. However, the amount of available heat for extra power generation by external integration, essential for the viability of this technology, is also reduced. This is the case of the configurations including a cyclonic preheater or a mixing seal valve. This study assesses the energy penalty minimization that may be reached by external integration of these internal energy integration configurations. A methodological process has been applied to obtain a reduction of the energy penalty with respect to the ordinary configuration. This energy saving combined with the lower size of equipment and reduced capital cost would make the cyclonic preheater the most suitable configuration to improve the viability of this technology.

17/02283 Historical variations in the stable isotope composition of mercury in a sediment core from a riverine lake: effects of dams, pulp and paper mill wastes, and mercury from a chlor-alkali plant

Jackson, T. A. *Applied Geochemistry*, 2016, 71, 86–98.

The Wabigoon River (Ontario, Canada) was affected by dams starting in 1898 and was polluted with pulp and paper mill wastes starting in 1913 and mercury from a chlor-alkali plant from 1962 to 1975. A dated sediment core from a riverine lake was analysed to investigate resultant changes in the biogeochemistry of mercury as revealed by variations in mercury isotope ratios and sediment chemistry. A total mercury maximum formed by the mercury pollution coincided with minimums in the δ-values of the $^{198}Hg/^{202}Hg$, $^{199}Hg/^{202}Hg$, $^{200}Hg/^{202}Hg$, and $^{201}Hg/^{202}Hg$ ratios, and the δ-values decreased in the order $\delta^{201}Hg > \delta^{200}Hg > \delta^{199}Hg > \delta^{198}Hg$. Thus, mass-dependent fractionation caused depletion in lighter isotopes, implying evaporation of Hg(0) and pollution of the atmosphere as well as the river-lake system. Concurrently, mass-independent fractionation caused ^{199}Hg enrichment, possibly reflecting an independently documented upsurge in methylmercury production, and ^{201}Hg depletion, suggesting removal of methylmercury with anomalously high $^{201}Hg/^{199}Hg$ ratios by aquatic organisms and accumulation of ^{201}Hg-depleted inorganic Hg(II) in sediments. The $\delta^{201}Hg/\delta^{199}Hg$ ratio rose abruptly when mercury pollution began, reflecting the resultant increase in methylmercury production, and remained high but gradually declined as the pollution abated, paralleling trends shown by methylmercury in aquatic organisms. The $\delta^{201}Hg/\delta^{199}Hg$ ratio of pre-1962 background mercury increased *ca.* 1898 and *ca.* 1913–1929, suggesting accelerated methylmercury production due to stimulation of microbial activities by the damming of the river and the input of pulp and paper mill wastes, respectively. Other variations were linked to economic and technological factors that affected pulp and paper manufacture.

17/02284 Integrated anaerobic ammonium oxidization with partial denitrification process for advanced nitrogen removal from high-strength wastewater

Cao, S. *et al. Bioresource Technology*, 2016, 221, 37–46.

In this study, a novel integrated anaerobic ammonium oxidization with partial denitrification process (termed as ANAMMOX-PD) was developed for advanced nitrogen removal from high-strength wastewater, which excess NO_3^--N produced by ANAMMOX was fed into PD reactor for NO_2^--N production and then refluxing to ANAMMOX reactor for further removal. Results showed that total nitrogen (TN) removal efficiency as high as 97.8% was achieved and effluent TN-N was below 20 mg/L at influent TN-N of 820 mg/L. Furthermore, the feasibility of simultaneously treating domestic wastewater was demonstrated in ANAMMOX-PD process, and NH_4^+-N removal efficiency of 96.7% was obtained. The nitrogen removal was mainly carried out through ANAMMOX pathway, and high-throughput sequencing revealed that *Candidatus* Brocadia was the major ANAMMOX species. The presented process could effectively solve the problem of excess nitrate residual in ANAMMOX effluent, which hold a great potential in application of currently ANAMMOX treating high-strength wastewater (e.g. sludge digestion supernatant).

17/02285 Interplay of inlet temperature and humidity on energy penalty for CO_2 post-combustion capture: rigorous analysis and simulation of a single stage gas permeation process

Giordano, L. *et al. Energy*, 2016, 116, 517–525.

Over the last decade, membrane separation processes have attracted considerable research attention. This is due to their potential for lowering the costs of post-combustion CO_2 capture compared with the more established technologies, which are based on the use of chemical solvents. It is well known that the performance of membrane-based CO_2 capture is related to several factors, including flue gas composition, membrane material and system design. Membrane working temperature is one of the operating parameters that have several implications on the CO_2 separation process. However, surprisingly, this key operating variable has not been investigated in detail. It not only influences the intrinsic membrane properties and the feed composition but also indirectly affects the energy behaviour of the whole capture system. Hence, the resulting outcome cannot be intuitively deduced. In this work the combined effect of operating temperature and humidity on a CO_2 capture process has been deeply investigated, focusing on a single stage membrane unit with feed compression and permeate vacuum pumping. Considering as case study the flue gas from a coal-fired power plant, the paper assesses the variation in separation performances with respect to CO_2 permeate purity and membrane area. The variation of energy expenses of membrane system with respect to two types of polymeric membranes (Polyactive 1500, PIM-1), which have different gas separation properties (permeability, selectivity), has also been evaluated. This study reveals that an increase in the membrane operating temperature from 30 to 70 °C negatively affects CO_2 permeate purity, losing more than 10% irrespective of capture

ratio. Conversely, the influence on area requirement is strictly related to the type of membrane material. Additionally the specific energy requirement to drive the separation process increases, ranging from around 250 kWh/tonne (Polyactive 1500) to 290 kWh/tonne (PIM-1) for a separation degree of 90%.

17/02286 Living walls and their contribution to improved thermal comfort and carbon emission reduction: a review

Charoenkit, S. and Yiemwattana, S. *Building and Environment*, 2016, 105, 82–94.

A growing number of living wall studies in the recent decade indicate the increasing interest in the environmental benefits of this greening system. Most studies focus on the energy benefits of the living walls that help to cool down the indoor spaces and reduce energy consumption and carbon emissions from the building sector. Living walls also have a carbon reducing benefit as they are able to sequester carbon dioxide (CO_2) in plant biomass and substrate. Living walls can therefore be considered as an important measure for climate mitigation in urban environments. Literature review was conducted to demonstrate thermal performances of the living walls in four climates: tropical, desert, temperate, and Mediterranean. The comparative analysis between living walls and green roofs was also undertaken to determine CO_2 sequestration performance of living walls. Influencing factors affecting thermal and CO_2 sequestration performances of living walls are highlighted and the research gaps needed to be addressed in each factor are pointed out. It was found that plant and substrate characteristics are the major factors that have impacts on both energy and CO_2 performance, but these two environmental benefits of living walls are separately examined. Finally, the recommendations are presented to promote the integration of both energy and CO_2 aspects in the future studies of living walls.

17/02287 Location matters: population density and carbon emissions from residential building energy use in the United States

Timmons, D. *et al. Energy Research & Social Science*, 2016, 22, 137–146.

This study considers how carbon emissions from US housing stock change with urban location and associated population density, using data from the US Residential Energy Consumption Survey (RECS) and American Community Survey (ACS) in a mediation model to quantify direct and indirect effects of population density on carbon emissions. Urban living in the USA today is generally associated with lower levels of residential carbon emissions, with some of the more significant effects being indirect. For example, more densely populated areas are associated with decreased housing size, which in turn decreases carbon emissions. One of the largest indirect effects observed is from the prevalence of natural gas heating in urban areas. Large indirect effects were also observed from the urban prevalence of attached and multi-family housing. A policy question is whether emissions-reducing housing choices could be effectively promoted in non-urban areas.

17/02288 Minimization of CO_2 capture energy penalty in second generation oxy-fuel power plants

Escudero, A. I. *et al. Applied Thermal Engineering*, 2016, 103, 274–281.

Oxy-combustion is one of the most promising technologies to reduce CO_2 emissions from coal-fired power plants. Nevertheless, as CO_2 capture system there is an important energy penalty and efficiency of the overall power plant substantially decreases. It is well accepted that the application of first generation post-combustion and oxy-fuel combustion technologies reduce the power plant efficiency in 10–12 efficiency points. Air separation unit (ASU) and compression and purification unit (CPU) are the main energy consumers in the oxy-fuel process. Moreover, the oxidant flow, which is a mixture of O_2 and recirculated flue gases (RFG), requires a high heating demand in order to preheat it before the boiler inlet. This paper presents a methodology for the minimization of the energy penalty in oxy-fuel power plants that also includes ASU and CPU optimized designs with lower energy consumption, a boiler working with a high oxygen concentration (up to $40\%_v$) in oxidant and waste energy integrated with a new designed steam cycle. Results show an important increase in power plant net efficiency (36.42%, LHV basis) regarding oxy-fuel reference power plant (32.91%). As a consequence, energy penalty can be reduced from original 10.5 points to 7.3 points.

17/02289 Nitrogen and phosphorus removal coupled with carbohydrate production by five microalgae cultures cultivated in biogas slurry

Tan, F. *et al. Bioresource Technology*, 2016, 221, 385–393.

In this study, five microalgae strains were cultured for their ability to survive in biogas slurry, remove nitrogen resources and accumulate carbohydrates. It was proved that five microalgae strains adapted in biogas slurry well without ammonia inhibition. Among them, *Chlorella vulgaris* ESP-6 showed the best performance on carbohydrate accumulation, giving the highest carbohydrate content of 61.5% in biogas slurry and the highest ammonia removal efficiency and rate of 96.3% and 91.7 mg/L/d respectively in biogas slurry with phosphorus and magnesium added. Additionally, the absence of phosphorus and magnesium that can be adverse for biomass accumulation resulted in earlier timing of carbohydrate accumulation and magnesium was firstly recognized and proved as the influence factor for carbohydrate accumulation. Microalgae that cultured in biogas slurry accumulated more carbohydrate in cell, making biogas slurry more suitable medium for the improvement of carbohydrate content, thus can be regarded as a new strategy to accumulate carbohydrate.

17/02290 Novel effect of SO_2 on selective catalytic oxidation of slip ammonia from coal-fired flue gas over IrO_2 modified Ce–Zr solid solution and the mechanism investigation

Chen, W. *et al. Fuel*, 2016, 166, 179–187.

The slip ammonia from selective catalytic reduction (SCR) of NO_x in coal-fired flue gas can cause degeneration of the utilities and environmental issues like aerosol. To achieve selective catalytic oxidation (SCO) of slip ammonia to N_2, novel IrO_2 modified Ce–Zr solid solution catalysts were synthesized and tested under various conditions. It was found that $IrO_2/Ce_{0.6}Zr_{0.4}O_2$ (PVP) catalyst displayed outstanding catalytic activity for slip ammonia and the removal efficiency was higher than 98%. Interestingly, the effect of SO_2 on NH_3 oxidation was bifacial, which the presence of SO_2 could result in slight deactivation of catalyst but also improve the N_2 selectivity of oxidized products to as high as 100% with coexistence of SO_2 and NH_3. The mechanism of NH_3-SCO process over $IrO_2/Ce_{0.6}Zr_{0.4}O_2$ (PVP) was evaluated through various techniques, and the results demonstrated that NH_3 oxidation could follow both –NH mechanism and internal SCR (iSCR) mechanism at different temperature regions. And the dominant pathway is the iSCR mechanism, in which adsorbed ammonia is firstly activated and reacts with oxygen atoms to form the –HNO intermediate. Then, the –HNO could be oxidized with atomic oxygen from O_2 to form NO species. Meanwhile, the formed/adsorbed NO could interact with $–NH_2$ to N_2 with N_2O as by-product, and the presence of SO_2 can effectively inhibit the production of N_2O and NO. Also, the mechanism of SO_2 effects was also evaluated and determined reasonably.

17/02291 On the modelling of multidisciplinary electrochemical systems with application on the electrochemical conversion of CO_2 to formate/formic acid

Georgopoulou, C. *et al. Computers & Chemical Engineering*, 2016, 93, 160–170.

This paper presents a model-based approach on the analysis of complex multidisciplinary electrochemical processes, with implementation on a reactor for the electrochemical conversion of CO_2 to formate/formic acid. The process is regarded as a system of interacting physical and electrochemical mechanisms. A process model is developed by combining individual mathematical sub-models of the mechanisms, organized at groups of compartments following the physical process structure. This approach results in a generic reconfigurable model that can be used as a part of integrated systems, and to test design modifications. The approach is demonstrated on an electrochemical cell, where CO_2 is converted to formate/formic acid. The model captures the molar transportation under electric field, the two-phase flow effects, and the key electrochemical reactions. The model is calibrated and validated against experimental data obtained from a continuous flow cell. The key parameters affecting the process performance are discussed through scale-up analysis.

17/02292 Patterns and determinants of household use of fuels for cooking: empirical evidence from sub-Saharan Africa

Rahut, D. B. *et al. Energy*, 2016, 117, 93–104.

The use of clean sources of energy for cooking is critical for securing better health for women and children and improving the overall standard of living of people in developing countries. Despite increasing awareness and the revolution in energy sources, a vast majority of households in developing countries continue to use solid fuels for cooking, which are considered to be harmful to both the environment and human health. This paper uses the World Bank's comprehensive living standard survey measurement data from Ethiopia, Malawi and Tanzania to analyse cooking fuel use patterns and their determinants. The descriptive analysis shows that a significant number of households use solid fuels for cooking and only a small fraction of households use clean fuels such as electricity, liquid petroleum gas. Rural households and those situated far from markets are more dependent on dirty fuels. Multinomial logit and ordered probit model estimation results show that female-headed households, household heads with a higher level of education, urban and wealthy households are more likely to use modern energy sources such as electricity and liquid petroleum gas, and are less likely to use solid fuels.

17/02293 Performance analysis of different scrubber systems for removal of particulate emissions from a small size biomass boiler

Bianchini, A. *et al. Biomass and Bioenergy*, 2016, 92, 31–39.

Biomass boiler plants of small thermal power (<35 kW thermal), in particular for domestic heating, have greatly contributed to the rise in particulate emissions. Several technologies, like fabric filters or electrostatic precipitators, can achieve high particulate removal efficiency, over 99%. However, the application of these technologies is limited by excessive prices and operational problems, since the high cost does not allow their use in small size plants. The paper shows a comparative performance analysis of different scrubber systems which have been designed, realized and tested with flue gas produced by biomass combustion in a 25 kW thermal boiler. The experimental campaigns were realized in the laboratory of the Department of Industrial Engineering of the University of Bologna. Experimental results demonstrate the achievements of particulate removal efficiency which is comparable with the efficiency of industrial technologies. Moreover, a preliminary energy balance was carried out to assess the energy cost of the different scrubber systems tested.

17/02294 Potassium promotion effects in carbon nanotube supported molybdenum sulfide catalysts for carbon monoxide hydrogenation

Liu, C. *et al. Catalysis Today*, 2016, 261, 137–145.

The paper focuses on the effect of potassium promotion on the structure and catalytic performance of carbon nanotube supported molybdenum sulfide catalysts for carbon monoxide hydrogenation. A combination of characterization techniques showed the presence of MoO_2 and mixed K-Mo oxides in the calcined catalysts. The sulfidation of oxide phases leads to MoS_2 and K-Mo sulfides. MoO_2 showed somewhat lower extent of sulfidation compared to other molybdenum oxide species. MoS_2 was principally responsible for CH_4 production, while lighter olefins, paraffins, alcohols and higher hydrocarbons were produced on the mixed K-Mo sulfides. The catalyst basicity seems to be one of the important factors controlling the reaction selectivity; moderate basicity is essential for higher rates of olefin and alcohol synthesis.

17/02295 Removal of CO from CO-contaminated hydrogen gas by carbon-supported rhodium porphyrins using water-soluble electron acceptors

Yamazaki, S.-i. *et al. Journal of Power Sources*, 2016, 329, 88–93.

Carbon-supported Rh porphyrins catalyse the oxidation of carbon monoxide by water-soluble electron acceptors. The rate of this reaction is plotted as a function of the redox potential of the electron acceptor. The rate increases with an increase in the redox potential until it reaches a plateau. This profile can be explained in terms of the electrocatalytic CO oxidation activity of the Rh porphyrin. The removal of CO from $CO(2\%)/H_2$ by a solution containing a carbon-supported Rh porphyrin and an electron acceptor is examined. The complete conversion of CO to CO_2 is achieved with only a slight amount of Rh porphyrins. Rh porphyrin on carbon black gives higher conversion than that dissolved in solution. This reaction can be used not only to remove CO in anode gas of stationary polymer electrolyte fuel cells but also to regenerate a reductant in indirect CO fuel cell systems.

17/02296 Satisfying light conditions: a field study on perception of consensus light in Dutch open office environments

Chraibi, S. *et al. Building and Environment*, 2016, 105, 116–127.

Workplace innovation has been changing the European office landscape into mostly open spaces, where enhanced interaction between people is combined by efficient use of space. However, challenges are found in offering individual preferred conditions in these multi-user spaces, especially when dealing with shared systems. Previous studies clearly show the benefits of personal control as a means to achieve individual preferred lighting. Most of these benefits were demonstrated in private offices or situations where users have a 'personal' light source. Lighting systems in open offices are often designed as a regular grid of luminaires to deliver uniform lighting. This often results in a luminaire grid that does not match the desk arrangement, making it challenging to offer personal lighting controls. By grouping luminaires, users could be offered consensus control. The question is whether consensus control brings advantages rather than disadvantages. This paper presents the results of a field study evaluating consensus light control in an open office. Fourteen users experienced a reference no-control condition and a condition with control over a zone of luminaires. Data were collected by objective measurements as well as subjective surveys and interviews. This study shows that consensus control in an open office improves satisfaction of individual users with the light quantity and quality. Even though the controllable light is shared, consensus among users results in an improved lighting environment for the majority of users. Selected illuminances in the condition with controls were on average lower than in the reference condition, resulting in lower energy usage by lighting.

17/02297 SO_2 flux and the thermal power of volcanic eruptions

Henley, R. W. and Hughes, G. O. *Journal of Volcanology and Geothermal Research*, 2016, 324, 190–199.

A description of the dynamics, chemistry and energetics governing a volcanic system can be greatly simplified if the expansion of magmatic gas can be assumed to be adiabatic as it rises towards the surface. The conditions under which this assumption is valid are clarified by analysis of the transfer of thermal energy into the low conductivity wallrocks traversed by fractures and vents from a gas phase expanding over a range of mass flux rates. Adiabatic behaviour is predicted to be approached typically within a month after perturbations in the release of source gas have stabilized, this timescale being dependent upon only the characteristic length scale on which the host rock is fractured and the thermal diffusivity of the rock. This analysis then enables the thermal energy transport due to gas release from volcanoes to be evaluated using observations of SO_2 flux with reference values for the $H_2O:SO_2$ ratio of volcanic gas mixtures discharging through high temperature fumaroles in arc and mantle-related volcanic systems. Thermal power estimates for gas discharge are $10^{1.8}$–$10^{4.1}\,MW_H$ during quiescent, continuous degassing of arc volcanoes and $10^{3.7}$–$10^{7.3}\,MW_H$ for their eruptive stages, the higher value being the Plinean Pinatubo eruption in 1991. Fewer data are available for quiescent stage mantle-related volcanoes (Kilauea $10^{2.1}\,MW_H$) but for eruptive events power estimates range from $10^{2.8}\,MW_H$ to $10^{5.5}\,MW_H$. These estimates of thermal power and mass of gas discharges are commensurate with power estimates based on the total mass of gas ejected during eruptions. The sustained discharge of volcanic gas during quiescent and short-lived eruptive stages can be related to the hydrodynamic structure of volcanic systems with large scale gaseous mass transfer from deep in the crust coupled with episodes of high level intrusive activity and gas release.

17/02298 Study of carbonaceous fractions associated with indoor $PM_{2.5}/PM_{10}$ during Asian cultural and ritual burning practices

Dewangan, S. *et al. Building and Environment*, 2016, 106, 229–236.

The study was carried out to evaluate the seasonal and annual trend of thermal fractions (organic and elemental carbon) associated to different cultural/ritual-indoor aerosol carbonaceous matter compared to residential-indoors and ambient-outdoors. Thermal speciation of carbonaceous fractions (SCFs: OC1, OC2, OC3, OC4, OP, EC1, EC2, EC3) associated to cultural/ritual-indoors and indoor/outdoor relationship were also taken into account in four different types of cultural/ritual centres: (1) marriage places (MP), (2) Muslim holy shrines (MHS), (3) Buddhist temples (BT) and (4) Hindu temples (HT). Longitudinally measured 360 $PM_{2.5}/PM_{10}$ samples throughout the year 2012–2013, onto quartz fibre filters, were analysed for organic (OC) and elemental carbon (EC) along with eight SCFs using thermal/optical reflectance/transmittance method. SCFs were determined in selected samples, representing all selected cultural/ritual-indoors, to address the source markers associated to biomass burning (BB) emissions; observed during cultural/ritual performances. Results have shown significantly higher levels of BB markers' SCFs in cultural/ritual-indoors compared those reported for residential-indoors and ambient-outdoors. Three to eight-fold higher carbonaceous aerosols was found in cultural/ritual-indoors compared to those determined in residential-indoors and ambient-outdoors. OC/EC ratio was found two-fold higher in MHS and MP places compared to those found in other selected indoor and outdoor sites. Similarly, higher degree of seasonal variability with higher occurrence of aerosol fractions and associated OC and EC in winter is observed in both MHS and MP due to higher activity pattern.

17/02299 Study of multi-twisted-tube gas cooler for CO_2 heat pump water heaters

Yang, Y. *et al. Applied Thermal Engineering*, 2016, 102, 204–212.

Multi-twisted-tube type heat exchangers applied in a transcritical CO_2 heat pump as gas coolers were investigated. The influence of different numbers of inner tubes on the heat transfer and the pressure drop was discussed by means of experiments and theoretical analysis. The performances of two gas coolers with three and four inner tubes were measured and compared. It is found that heat transfer characteristics of the gas cooler with four inner tubes is better than that with three inner tubes. Based on the theoretical analysis, outlet temperature of water increases with increasing the number of inner tubes at the beginning and the increasing tendency becomes gentle when the number of inner tubes is more than four. But the pressure drop of gas cooler rises greatly with the increment of the number of inner tubes. It is implied from the analysis that the coefficient of performance of CO_2 heat pump is not optimum when the outlet temperature of water

becomes high by increasing mass flow rate of CO_2 and decreasing the mass flow rate of water. In order to get both high COP and high outlet temperature of water, the water side heat transfer coefficient of the gas cooler needs improving.

17/02300 Techno-economic process design of a commercial-scale amine-based CO_2 capture system for natural gas combined cycle power plant with exhaust gas recirculation

Ali, U. *et al. Applied Thermal Engineering*, 2016, 103, 747–758.

Post-combustion CO_2 capture systems are gaining more importance as a means of reducing escalating greenhouse gas emissions. Moreover, for natural gas-fired power generation systems, exhaust gas recirculation is a method of enhancing the CO_2 concentration in the lean flue gas. The present study reports the design and scale-up of four different cases of an amine-based CO_2 capture system at 90% capture rate with 30 wt% aqueous solution of monoethanolamine. The design results are reported for a natural gas-fired combined cycle system with a gross power output of 650 MW_e without exhaust gas recirculation (EGR) and with EGR at 20%, 35% and 50% EGR percentage. A combined process and economic analysis is implemented to identify the optimum designs for the different amine-based CO_2 capture plants. For an amine-based CO_2 capture plant with a natural gas-fired combined cycle without EGR, an optimum liquid-to-gas ratio of 0.96 is estimated. Incorporating EGR at 20%, 35% and 50%, results in optimum liquid to gas ratios of 1.22, 1.46 and 1.90, respectively. These results suggest that a natural gas-fired power plant with exhaust gas recirculation will result in lower penalties in terms of the energy consumption and costs incurred on the amine-based CO_2 capture plant.

17/02301 The effect of steam on a synthetic Ca-based sorbent for carbon capture

González, B. *et al. Chemical Engineering Journal*, 2016, 285, 378–383.

The rate and extent of a synthetic sorbent containing 83 wt% CaO, 14 wt% MgO and 3 wt% $Ca_{12}Al_{14}O_{33}$ to react with CO_2 at ~750 °C was investigated in the presence of 5 or 10 vol% steam. Similar to the natural sorbents and their derivatives, the rate and extent of carbonation by the synthetic sorbent was found to increase substantially with the partial pressure of steam. This improvement appears to be due to the ability of steam to promote the growth of product islands of $CaCO_3$ in the direction normal to the surface, as well as affecting the porosity of the calcined material.

Hydrocarbon emissions

17/02302 A novel approach for apportionment between primary and secondary sources of airborne nitrated polycyclic aromatic hydrocarbons (NPAHs)

Lin, Y. *et al. Atmospheric Environment*, 2016, 138, 108–113.

Nitrated polycyclic aromatic hydrocarbons (NPAHs) are strong environmental mutagens and carcinogens originating from both primary emissions and secondary reactions in the atmosphere. The sources and the toxicity of different NPAH species could vary greatly; therefore a specie-specific source apportionment is essential to evaluate their health risks and to formulate controlling regulations. However, few studies have reported source apportionment of NPAHs species to date. This study developed an easy-to-perform method for the apportionment of primary versus secondary sources of airborne NPAHs based on the relationship between NPAHs and NO_2. After log-transformation of both NPAHs and NO_2 concentrations, a slope of β between these two variables was obtained by the linear regression. When β is significantly smaller than 1, it indicates primary emissions while β significantly greater than 1 suggests secondary formation. The authors have validated this method with data previously collected in Beijing. A good correlation, with R value of 0.57, was observed between results produced by this new method and by positive matrix factorization. The correlation could be further improved ($RI = 0.71$) if the gas/particle partition of NPAHs is taken into consideration. This developed method enables the source apportionment for individual NPAHs species and could be used to validate the results of other receptor models.

17/02303 A refined method for the calculation of the non-methane volatile organic compound emission estimate from domestic solvent usage in Ireland from 1992 to 2014 – a case study for Ireland

Barry, S. and O'Regan, B. *Atmospheric Environment*, 2016, 138, 15–21.

This study describes a new methodology to calculate non-methane volatile organic compounds from domestic solvent use including fungicides over the period 1992–2014. Improved emissions data compiled at a much more refined level can help policy-makers develop more effective policy's to address environmental issues. However, a number of problems were found when member states attempt to use national statistics for domestic solvent use including fungicides. For instance, the European Monitoring and Evaluation Programme/ European Environment Agency's Air Pollutant Emission Inventory Guidebook provides no guidance regarding which activity data should be used, resulting in emission estimates being potentially inconsistent and uncomparable. Also, previous methods and emission factors described in the Air Pollutant Emission Inventory Guidebook do not exactly match data collected by state agencies. This makes using national statistics difficult. In addition, the Air Pollutant Emission Inventory Guidebook uses broader categories than necessary (e.g. cosmetics aerosol/non-aerosol) to estimate emissions while activity data is available at a more refined level scale (e.g. personal cleaning products, hair products, cosmetics, deodorants and perfumes). This can make identifying the drivers of emissions unclear. This study builds on an earlier one whereby it provides a method for collecting activity data from state statistics, developed country specific emission factors based on a survey of 177 Irish products and importantly, used a new method to account for the volatility of organic compounds found in commonly available domestic solvent containing products. This is the first study to account for volatility based on the characteristics of organic compounds and therefore is considered a more accurate method of accounting for emissions from this emission source. The results of this study can also be used to provide a simple method for other member parties to account for the volatility of organic compounds using sectorial adjustment factors described here. For comparison purposes, emission estimates were calculated using the Tier 1 approach currently used in the emission inventory, using activity data and emission factors unadjusted for volatility and adjusted for volatility. The unadjusted estimate is useful, because it demonstrates the failure to properly account for volatility can produce significantly over-estimated emissions from the domestic solvent usage sector. Unadjusted emissions were found to be 30% lower than the Air Pollutant Emission Inventory Guidebook Tier 1 period in 2014. Emissions were found to reduce a further 20.9% when the volatility of the organic compounds was included. This new method shows that member parties may be significantly overestimating emissions from domestic solvent use including pesticides and further work should include refining organic compound content and the sectorial adjustment factor of products.

17/02304 Analytical solution of VOCs emission from wet materials with variable thickness

Deng, B. *et al. Building and Environment*, 2016, 104, 145–151.

Volatile organic compound (VOC) emissions from wet materials lead to the movement of the material–air interface with time. A transient diffusion equation with moving boundary is developed to describe VOCs emission from wet materials. A coordinate transform technique is presented to transfer the moving boundary problem into a fixed boundary problem. The generalized integral transform technique is used to obtain an analytical solution of the fixed boundary problem. An environmental chamber test on formaldehyde emission from oil-based paint is performed to validate the present model. Results of the present model agree well with the experimental data. The influence of parameters on the emission of formaldehyde is discussed. With the increase of diffusion coefficient, the VOCs emission rate increases. On the contrary, with the increase of partition coefficient, the VOCs emission rate decreases. The present model can be used to predict the emission of VOCs from wet coating materials with variable thickness.

17/02305 Aromatic compound emissions from municipal solid waste landfill: emission factors and their impact on air pollution

Liu, Y. *et al. Atmospheric Environment*, 2016, 139, 205–213.

Aromatic compounds (ACs) are major components of volatile organic compounds emitted from municipal solid waste (MSW) landfills. The ACs emissions from the working face of a landfill in Beijing were studied from 2014 to 2015 using a modified wind tunnel system. Emission factors (EFs) of fugitive ACs emissions from the working face of the landfill were proposed according to statistical analyses to cope with their uncertainty. And their impacts on air quality were assessed for the first time. Toluene was the dominant AC with an average emission rate of $38.8 \pm 43.0\,\mu g\,m^{-2}\,s^{-1}$ (at a sweeping velocity of $0.26\,m\,s^{-1}$). An increasing trend in AC emission rates was observed from 12:00 to 18:00 and then peaked at 21:00 ($314.3\,\mu g\,m^{-2}\,s^{-1}$). The probability density functions (PDFs) of AC emission rates could be classified into three distributions: Gaussian, log-normal, and logistic. EFs of ACs from the working face of the landfill were proposed according to the 95th percentile cumulative emission rates and the wind effects on ACs emissions. The annual ozone formation and secondary organic aerosol formation potential caused by AC emissions from landfills in Beijing were estimated to be $8.86 \times 10^5\,kg\,year^{-1}$ and $3.46 \times 10^4\,kg\,year^{-1}$, respectively. Toluene, $m + p$-xylene, and 1,3,5-trimethylbenzene were the most significant contributors to air pollution. Although ACs pollutions from landfills accounts for less

percentage (~0.1%) compared with other anthropogenic sources, their fugitive emissions which cannot be controlled efficiently deserve more attention and further investigation.

17/02306 Diurnal variation of particle-bound PAHs in an urban area of Spain using TD-GC/MS: influence of meteorological parameters and emission sources

Elorduy, I. *et al. Atmospheric Environment*, 2016, 138, 87–98.

Short-term particulate concentrations of 13 polycyclic aromatic hydrocarbons (PAHs) in PM_{10} were determined in the urban area of Bilbao, Spain. The analysis was performed by thermal desorption coupled with gas chromatography-mass spectrometry, which enabled to use three diurnal periods of 8 h sampling basis time resolution. A total of 105 PM_{10} samples were collected during 5 months in 2013. Diurnal average concentration of total PAHs (Σ13 PAHs) ranged from 1.18 to 9.78 ng m^{-3}; and from 0.06 to 0.70 ng m^{-3} for benzo[*a*]pyrene. The presence of high concentrations of benzo[*b*]fluoranthene, pyrene, fluoranthene and chrysene, and the significant PAHs diurnal variations due to the sampling period, pointed out the influence of mixing anthropogenic sources and meteorological conditions. The diurnal pattern of source contributions was assessed by binary diagnostic ratios and principal component analysis (PCA). These results showed the prevalence of pyrogenic sources coming from traffic and coal/coke combustion sources. Moreover, the PCA differentiated a diurnal pattern of source contributions. The influence of meteorological factors was studied by Pearson correlation analysis and multiple linear regression. Three factors, temperature, wind speed and atmospheric pressure, were identified as the most significant ones affecting diurnal PAHs concentrations. Finally, PCA of the PAHs levels, regulated atmospheric pollutants and meteorological parameters showed that diurnal PAHs concentrations were mainly influenced by variations in the emission sources, atmospheric oxidants such as ozone, and temperature conditions. These results provide further insight into the PAHs diurnal patterns in urban areas by using higher temporal resolutions.

17/02307 Measurements and source apportionment of particle-associated polycyclic aromatic hydrocarbons in ambient air in Riyadh, Saudi Arabia

Bian, Q. *et al. Atmospheric Environment*, 2016, 137, 186–198.

Ambient air samples were obtained in Riyadh, the capital and largest city of Saudi Arabia, during two measurement campaigns spanning September 2011 to September 2012. Sixteen particle-phase polycyclic aromatic hydrocarbons (PAH) were quantified in 167 samples. Pyrene and fluoranthene were the most abundant PAH, with average of 3.37 ± 14.01 and 8.00 ± 44.09 ng m^{-3}, respectively. A dominant contribution from low molecular weight (LMW) PAH (MW < 228) suggested a large influence of industrial emissions on PAH concentrations. Monte Carlo source apportionment using diagnostic ratios showed that $80 \pm 10\%$ of the average LMW PAH concentrations were contributed by petroleum vapour emissions, while $53 \pm 19\%$ of high molecular weight (HMW) PAH were from solid fuel combustion emissions. The positive matrix factorization model estimated that oil combustion emissions dominated total PAH concentrations, accounting for on average 96%, likely due to widespread use of oil fuels in energy production (power plants and industries). The results demonstrate the significant influence of petroleum product production and consumption on particulate-phase PAH concentrations in Riyadh, but also point to the importance of traffic and solid fuel burning, including coke burning and seasonal biomass burning, especially as they contribute to the ambient levels of HMW PAH.

17/02308 Spatio-temporal variations and influencing factors of polycyclic aromatic hydrocarbons in atmospheric bulk deposition along a plain-mountain transect in western China

Xing, X. *et al. Atmospheric Environment*, 2016, 139, 131–138.

Ten atmospheric bulk deposition (the sum of wet and dry deposition) samplers for polycyclic aromatic hydrocarbons (PAHs) were deployed at a plain-mountain transect (namely PMT transect, from Daying to Qingping) in Chengdu Plain, West China from June 2007 to June 2008 in four consecutive seasons (about every 3 months). The bulk deposition fluxes of Σ_{15}-PAHs ranged from 169.19 to 978.58 μg m^{-2} yr^{-1} with geometric mean of 354.22 μg m^{-2} yr^{-1}. The most prevalent PAHs were four-ring (39.65%) and three-ring (35.56%) PAHs. The flux values were comparable to those in rural areas. Higher fluxes of total PAHs were observed in the middle of PMT transect (SL, YX and JY, which were more urbanized than other sites). The seasonal deposition fluxes in the sampling profile indicated seasonality of the contaminant source was an important factor in controlling deposition fluxes. PAHs bulk deposition was negatively correlated with meteorological parameters (temperature, wind speed, humidity, and precipitation). No significant correlations between soil concentrations and atmospheric deposition were found along this transect. PAHs in soil samples had combined sources of coal, wood and petroleum combustion, while a simple source of coal, wood and grass combustion for bulk deposition. There were significant positive correlation relationship ($p < 0.05$) between annual atmospheric bulk deposition and local PAHs emission, with biomass burning as the major contribution to the total emission of PAHs. This transect acts as an important PAHs source rather than being a sink according to the ratio of deposition/emission. Mountain cold trap effect existed in this transect where the altitude was higher than 1000 m. Long-range transport had an impact on the bulk deposition in summer. And this transect was a source to Tibetan only in summer. The forward trajectory analysis showed most air masses did not undergo long-range transport due to the blocking effect of surrounding mountains. Only a few air masses (<10%) arrived at the eastern and northern region of China or farther regions via long-range transport.

17/02309 The impact of fuel compositions on the particulate emissions of direct injection gasoline engine

Wang, Y. *et al. Fuel*, 2016, 166, 543–552.

An experimental study of particulate matter emissions was conducted on a direct injection gasoline (DIG) engine produced by a Chinese original equipment manufacturer (OEM) to investigate the impacts of fuel properties from China market on particulate emissions of modern gasoline vehicles. The emissions include both the primary emissions and the secondary ones in the atmosphere. The objective of this work is to provide some experimental data and analysis on the impacts of fuel properties and vehicle technologies on particulate matter-2.5 (PM2.5) in China. On the basis of better understanding of those impacts, it is desired to provide some suggestions and guidelines on how to improve fuel quality and vehicle technology to help effectively reduce air pollution in China. In this paper, six test fuels with different aromatics, olefin, sulfur, methyl-cyclopentadienyl manganese tricarbonyl (MMT), ethanol content were blended and tested to research on the influences on primary particulate emission including mass, number, size distribution and compounds including polycyclic aromatic hydrocarbons (PAHs) and the toxicity of PAHs emissions. The test results demonstrated that the fuel compositions impacted significantly on particulate emissions of DIG engine. Higher aromatics in gasoline resulted in much higher particle mass (PM), particle number (PN) and PAHs emission and much higher toxicity to human health. Reducing olefin content in gasoline showed benefits to a certain degree on reducing PM and PN emission especially under high load engine operation conditions, and did not show obvious improvement of PAHs emission factor, but reduced the toxicity of PAHs. 10% of Ethanol in gasoline showed limited improvement on particulate emissions comparing with the effect of reducing aromatics and olefin content in gasoline, moreover E10 increased PN emission under low load conditions. The test results also demonstrated that the typical China Phase V gasoline did not show benefits of reducing vehicle emissions the typical Phase IV gasoline with higher sulfur (≤50 ppm) and manganese (≤8 mg Mn/l) in China market. The particulate compounds of DIG engine mainly consisted elemental carbon (EC), organic matter (OM) and small amount of inorganic ions. The mass percentage of EC in total PM increased as the load of engine rose. Three-way catalyst (TWC) is more effective in reducing OM than EC, with the overall OM reduction rate of 67–85%.

Life cycle analysis

17/02310 An integrated life cycle sustainability assessment of electricity generation in Turkey

Atilgan, B. and Azapagic, A. *Energy Policy*, 2016, 93, 168–186.

This paper presents for the first time an integrated life cycle sustainability assessment of the electricity sector in Turkey, considering environmental, economic and social aspects. Twenty life cycle sustainability indicators (11 environmental, three economic and six social) are used to evaluate the current electricity options. Geothermal power is the best option for six environmental impacts but it has the highest capital costs. Small reservoir and run-of-river power has the lowest global warming potential while large reservoir is best for the depletion of elements and fossil resources, and acidification. It also has the lowest levelized costs, worker injuries and fatalities but provides the lowest life cycle employment opportunities. Gas power has the lowest capital costs but it provides the lowest direct employment and has the highest levelized costs and ozone layer depletion. Given these trade-offs, a multi-criteria decision analysis has been carried out to identify the most sustainable options assuming different stakeholder preferences. For all the preferences considered, hydropower is the most sustainable option for Turkey, followed by geothermal and wind electricity. This work demonstrates the importance for energy policy of

an integrated life cycle sustainability assessment and how tensions between different aspects can be reconciled to identify win–win solutions.

17/02311 Compression ignition of low-octane gasoline: life cycle energy consumption and greenhouse gas emissions
Hao, H. *et al. Applied Energy*, 2016, 181, 391–398.
The use of low-octane gasoline on gasoline compression ignition (GCI) engines is considered as a competitive alternative to the conventional vehicle propulsion technologies. In this study, a process-based, well-to-wheel conceptualized life cycle assessment model is established to estimate the life cycle energy consumption and greenhouse gas (GHG) emissions of the conventional gasoline–spark ignition (SI) and low-octane gasoline–GCI pathways. It is found that compared with the conventional pathway, the low-octane gasoline–GCI pathway leads to a 24.6% reduction in energy consumption and a 22.8% reduction in GHG emissions. The removal of the isomerization and catalytic reforming units in the refinery and the higher energy efficiency in the vehicle use phase are the substantial drivers behind the reductions. The results indicate that by promoting the use of low-octane gasoline coupled with the deployment of GCI vehicles, considerable reductions of energy consumption and GHG emissions in the transport sector can be achieved. However, significant technical and market barriers are still to be overcome. The inherent problems of NO_x and particulate matter exhaust emissions associated with GCI engines need to be further addressed with advanced combustion techniques. Besides, the yield of low-octane gasoline needs to be improved through adjusting the refinery configurations.

17/02312 Life cycle assessment of common reed (*Phragmites australis (Cav) Trin. ex Steud*) cellulosic bioethanol in Jiangsu Province, China
Shuai, W. *et al. Biomass and Bioenergy*, 2016, 92, 40–47.
Common reed (*Phragmites australis (Cav) Trin. ex Steud*) at wetlands is a natural resource in Jiangsu Province, China. Proper application of common reed could supplement bioenergy feedstocks and encourage wetlands conservation in this area. In this study, common reed and soil samples from wetlands near to farm, coastline and for wastewater treatment were collected. Potential bioethanol yield was estimated based on biomass yield and bioethanol production, and a life cycle assessment (LCA) model was built to analyse environmental performance of common reed bioethanol. The dry biomass yield of common reed was in the range of 3.8–36 $Mg\,ha^{-1}$, and location was the significant factor on biomass yield. Soil pH and available N content had positive impacts on yields of biomass and bioethanol; higher glucan content was detected in stem than in leaf and flower, while ash and klason lignin contents were higher in leaf than in stem and flower. The results indicated that wetlands with high available N content were very suitable for common reed growth, and stem fraction was better than leaf for bioethanol production. Based on LCA model calculation, the net energy and ratio of energy efficiency were compatible to bioethanol from switchgrass and rice straw, and the greenhouse gas emissions intensity and eutrophication potential were 15 $gCO_{2,eq}\,MJ^{-1}$ and $-1.1\,gPO_4^{3-}{}_{eq}\,MJ^{-1}$. The results indicate that common reed is a sustainable and renewable resource for bioethanol production, especially those grown on wetlands near to farmland in Jiangsu Province, China.

17/02313 Life cycle assessment of microalgae-based aviation fuel: influence of lipid content with specific productivity and nitrogen nutrient effects
Guo, F. *et al. Bioresource Technology*, 2016, 221, 350–357.
The aim of this work is to compare the life cycle assessments of low-N and normal culture conditions for a balance between the lipid content and specific productivity. In order to achieve the potential contribution of lipid content to the life cycle assessment, this study established relationships between lipid content (nitrogen effect) and specific productivity based on three microalgae strains including *Chlorella*, *Isochrysis* and *Nannochloropsis*. For microalgae-based aviation fuel, the effects of the lipid content on fossil fuel consumption and greenhouse gas (GHG) emissions are similar. The fossil fuel consumption (0.32–0.68 $MJ \cdot MJ^{-1}$ MBAF) and GHG emissions (17.23–51.04 $g\,CO_2e \cdot MJ^{-1}$ MBAF) increase (59.70–192.22%) with the increased lipid content. The total energy input decreases (2.13–3.08 $MJ \cdot MJ^{-1}$ MBAF, 14.91–27.95%) with the increased lipid content. The life cycle assessment indicators increased (0–47.10%) with the decreased nitrogen recovery efficiency (75–50%).

17/02314 The air emission assessment of a South Korean traditional building during its life cycle
Sim, J. and Sim, J. *Building and Environment*, 2016, 105, 283–294.
During its entire life cycle, a Korean traditional building produces various types of air emissions from the building material production, construction, operation, maintenance, demolition, and recycling and disposal stages, along with related transportation activities. This study investigates the life cycle air emissions of a building of this type located in Seoul, South Korea. The results of this study demonstrate that it produces 143,843.7 kg of CO_2, 1466.01 kg of CO, 686.22 kg of NO_X, 475.99 kg of SO_2, 280.59 kg of NMVOC, 274.44 kg of CH_4, and 1.26 kg of N_2O during its 30-year life span. In comparison with an apartment building, a traditional building significantly reduces about 98% of CO, 87% of CO_2, 78% of CH_4, 62% of NO_X, 45% of N_2O, and 36% of SO_2, except NMVOC emissions, in terms of life cycle air emission productivity. In addition, an environmental impact analysis of the building materials used finds that the roof tile has the largest impact on global warming potential, while the cement has the largest impact on ozone depletion potential.

16 ENERGY

Supplies, policy, economics, forecasts

17/02315 Access to electricity in the World Energy Council's global energy scenarios: an outlook for developing regions until 2030
Panos, E. *et al. Energy Strategy Reviews*, 2016, 9, 28–49.
Approximately two out of 10 people in the world still live without access to electricity. The United Nations 'Sustainable Energy to All – SE4All' initiative aims at eradicating this electricity access deficit by 2030. To estimate the financial effort required to achieve this target the authors analysed two long-term scenarios developed by the Paul Scherrer Institute and the World Energy Council, which describe two alternative economic and energy system developments. They focused on developing Asia, Latin America and Sub-Saharan Africa, which currently have the largest percentage of population without access to electricity. A long-term energy system model was then coupled with regional econometric models that forecasted population electrification rates. It was found that establishing universal electricity access by 2030 requires significant, but attainable investments in power generation infrastructure, and results in low impacts on primary energy demand and CO_2 emissions.

17/02316 Assessment of socioeconomic costs to China's air pollution
Xia, Y. *et al. Atmospheric Environment*, 2016, 139, 147–156.
Particulate air pollution has had a significant impact on human health in China and it is associated with cardiovascular and respiratory diseases and high mortality and morbidity. These health impacts could be translated to reduced labour availability and time. This paper utilized a supply-driven input–output (I–O) model to estimate the monetary value of total output losses resulting from reduced working time caused by diseases related to air pollution across 30 Chinese provinces in 2007. Fine particulate matter ($PM_{2.5}$) pollution was used as an indicator to assess impacts to health caused by air pollution. The developed I–O model is able to capture both direct economic costs and indirect cascading effects throughout inter-regional production supply chains and the indirect effects greatly outnumber the direct effects in most Chinese provinces. The results show the total economic losses of 346.26 billion Yuan (approximately 1.1% of the national gross domestic product, GDP) based on the number of affected Chinese employees (72 million out of a total labour population of 712 million) whose work time in years was reduced because of mortality, hospital admissions and outpatient visits due to diseases resulting from $PM_{2.5}$ air pollution in 2007. The loss is almost the annual GDP of Vietnam in 2010. The proposed modelling approach provides an alternative method for health-cost measurement with additional insights on inter-industrial and inter-regional linkages along production supply chains.

17/02317 China's carbon emissions embodied in (normal and processing) exports and their driving forces, 2006–2012
Su, B. and Thomson, E. *Energy Economics*, 2016, 59, 414–422.
This paper constructed a time-series extended input–output dataset (2006–2012) to analyse China's carbon emissions embodied in both normal and processing exports at a detailed 135-sector level. The structural decomposition analysis (SDA) was further applied to shed light on the driving forces behind the changes in their embodied emissions over the entire time period. This empirical study confirms the importance of using the extended model for analysing the trade-related embodiment, especially for processing exports. The embodied emissions in both normal and processing exports first increased from 2006 to 2008, then dropped during the global financial crisis (2008–2009), and then rose again after 2009. The embodied emissions as a percentage of total CO_2 emissions were quite stable before and after

the global financial crisis, at around 24% over the 2006–2008 period, and 18% over the 2010–2012 period. From 2006 to 2012, emission intensity played the key role in reducing the embodied emissions (around 595 Mt CO_2), while the total export effect contributed the most to the increase in embodied emissions (around 552 Mt CO_2). Similar analysis can be applied to other indicators, such as energy, water, greenhouse gas emissions, pollutants and materials.

17/02318 Economics of modern energy boomtowns: do oil and gas shocks differ from shocks in the rest of the economy?
Tsvetkova, A. and Partridge, M. D. *Energy Economics*, 2016, 59, 81–95.
The US shale boom has intensified interest in how the expanding oil and gas sector affects local economic performance. Research has produced mixed results and has not compared how energy shocks differ from equal-sized shocks elsewhere in the economy. What emerges is that the estimated impacts of energy development vary by region, empirical methodology, as well as the time horizon that is considered. This paper captures these dimensions to present a more complete picture of energy boomtowns. Utilizing US county data, the authors estimate the effects of changes in oil and gas extraction employment on total employment growth as well as growth by sector. They then compare this to the effects of equal-sized shocks in the rest of the economy to assess whether energy booms are inherently different. The analysis is performed separately for non-metropolitan and metropolitan counties using instrumental variables. The difference is considered over 1-, 3-, 6-, and 10-year time periods to account for county-fixed effects and to assess responses across different time horizons. The results show that in non-metropolitan counties, energy sector multiplier effects on total county employment first increase up to 6-year horizons and then decline for 10-year horizons. Positive spillovers were also observed to the non-traded goods sector, while spillovers were small or negative for traded goods. In metropolitan counties, there were no significant effects on total employment, although positive spillovers were present in some sectors. Yet, equal-sized shocks in the rest of the economy produced more jobs on average than oil and gas shocks, suggesting that policymakers should seek more diversified development.

17/02319 The new open flexible emission inventory for Greece and the greater Athens area (FEI-GREGAA): account of pollutant sources and their importance from 2006 to 2012
Fameli, K.-M. and Assimakopoulos, V. D. *Atmospheric Environment*, 2016, 137, 17–37.
Photochemical and particulate pollution problems persist in Athens as they do in various European cities, despite measures taken. Although, for many cities, organized and updated pollutant emissions databases exist, as well as infrastructure for the support of policy implementation, this is not the case for Greece and Athens. So far abstract efforts to create inventories from temporal and spatial annual low resolution data have not lead to the creation of a useful database. The objective of this study was to construct an emission inventory in order to examine the emission trends in Greece and the greater Athens area for the period 2006–2012 on a spatial scale of 6×6 and $2 \times 2\,km^2$, respectively, and on a temporal scale of 1 h. Emissions were calculated from stationary combustion sources, transportation (road, navigation and aviation), agriculture and industry obtained from official national and European sources. Moreover, new emission factors were calculated for road transport and aviation. The final database named FEI–GREGAA (Flexible Emission Inventory for GREece and the GAA) is open-structured so as to receive data updates, new pollutants, various emission scenarios and/or different emission factors and be transformed for any grid spacing. Its main purpose is to be used in applications with photochemical models to contribute to the investigation on the type of sources and activities that lead to the configuration of air quality. Results showed a decreasing trend in CO, NO_x and VOCs-NMVOCs emissions and an increasing trend from 2011 onwards in PM_{10} emissions. Road transport and small combustion contribute most to CO emissions, road transport and navigation to NO_x and small combustion and industries to PM_{10}. The onset of the economic crisis can be seen from the reduction of emissions from industry and the increase of biomass burning for heating purposes.

17/02320 Towards European targets by monitoring the energy profile of the Cyprus housing stock
Serghides, D. K. *et al. Energy and Buildings*, 2016, 132, 130–140.
Energy-efficient renovation of the existing housing stock is imperative to reduce building energy consumption since the building sector in Europe accounts for an estimated 40% of the energy used from all sectors and more than 80% of the buildings today will still exist in 2020. Following Europe's energy objectives, the paper investigates, based on the EU directives, the current energy refurbishment rates and examines the future energy performance of the Cyprus housing stock, in order to determine if they are adequate in achieving the Europe energy targets. The research focuses on pilot houses in Cyprus, which include dwellings from all typologies as classified, according to the IEE project EPISCOPE. The houses were monitored and based on the collected data and the performed simulations, their current and future energy performance are presented in the form of energy performance indicators. From the study, it is observed that with the current trends the national climate protection energy targets are unattainable. This is mainly due to the inadequate rate and depth of energy refurbishment of the existing housing stock and the ineptness of the Directives to address effectively the reduction of the cooling energy needs in the new constructions.

Energy conservation

17/02321 3D numerical thermal optimization of the roofs constructed with cast-in-situ hollow concrete floor system by finite volume method
Shi, G. Z. *et al. Energy and Buildings*, 2016, 131, 142–152.
Three-dimensional (3D) numerical thermal simulation on conjugate heat transfer in hollow roofs is conducted by self-compiled programme based on the finite volume method to improve insulation performance. Eight kinds of hollow roofs with different box fillers are optimized by regularly designing partitions to divide air-filled cavity. In addition, the effect of box filler materials on thermal behaviour is considered. The numerical results demonstrate that: horizontal partitions decrease the equivalent thermal conductivity by 13.65–40.42%, whose effect is more remarkable for higher void roofs, whereas vertical partitions cause few effects. Besides, different box filler materials can bring about slight variation no more than 3%.

17/02322 A framework for sensitivity analysis of data errors on home energy management system
Choi, D.-H. and Xie, L. *Energy*, 2016, 117, 166–175.
This paper investigates the impact of data errors on home energy management systems (HEMSs) that reduce energy cost and maintain comfort for residential consumers. In particular, a sensitivity analysis was conducted of HEMS subject to various types of input data such as the predicted energy consumption, the forecasted outdoor temperature, the consumers' comfort settings, static and dynamic operation constraints for home appliances, and the demand response (DR) signal. Using the perturbed Karush–Kuhn–Tucker (KKT) condition equations from the HEMS optimization formulation, the authors developed a linear sensitivity matrix to assess the impact of data on optimal solutions for: (1) electricity cost; (2) consumer's dissatisfaction cost; (3) the energy consumption for home appliances; and (4) the indoor temperature. The results of a simulation study using the developed sensitivity matrix provide HEMS operators with unique insight into factors that account for the relationships of HEMS operations to the change in the various data. Furthermore, these results can be used to provide insights for residential consumers and to evaluate the security risks of HEMS to cyberattacks through data manipulation.

17/02323 A novel surrogate model to support building energy labelling system: a new approach to assess cooling energy demand in commercial buildings
Melo, A. P. *et al. Energy and Buildings*, 2016, 131, 233–247.
Researchers in many countries are developing surrogate models to estimate the energy performance of the building stock. In Brazil, the building energy labelling system can be performed using a simplified method which is based on a basic surrogate model using multiple linear regressions. Based on the limitations associated with this model the aim of this study was to develop a more accurate surrogate model to predict the annual cooling energy demand of commercial buildings. The combination of all possible variations of the properties and their values resulted in more than 2.5 quadrillion cases. One million cases sampled by Latin hypercube method were considered. Several statistical modelling techniques were tested to generate the surrogate model: multiple linear regression, multivariate adaptive regression splines, support vector machines, the Gaussian process, random forests and artificial neural networks. The surrogate model was applied into a medium office to observe the difference between building energy simulation results. The results showed that the artificial neural network method presented the best performance, with a normalized root-mean-square deviation $<1\%$. The validation procedure indicates that the novel surrogate model is able to describe the relation between inputs data and cooling energy demand.

17/02324 Comparative study of energy saving potential for heavy chemical complex by area-wide approach
Matsuda, K. *Energy*, 2016, 116, 1397–1402.

The thought of single-site approach for energy saving in a site has been evolved to that of area-wide approach which considers multiple sites together as if they were a single entity. In area-wide approach, R-curve analysis plays an important part to evaluate the energy efficiency of the site utility system for utilizing high temperature heat, which is possible to identify energy saving potential and understand the characteristics of the utility system. R-curve analysis was applied to Mizushima complex, one of the ten largest heavy chemical complexes in Japan, and identified the characteristics and the energy saving potential for the whole of the complex. In area-wide approach, low-grade heat utilization for energy saving is also important. Total site profile analysis was used to evaluate the possibility of low-grade heat utilization. Mizushima complex was evaluated for the characterization by comparison of its energy saving potential to that of another heavy chemical complex, Chiba. It was found that the energy saving potential of Mizushima complex was twice in R-curve analysis than that of Chiba complex. This meant that the equipment in the utility system in Mizushima complex performed less efficiency than that in Chiba complex.

17/02325 Configuration of inter-city high-speed passenger transport infrastructure with minimal construction and operational energy consumption: a superstructure based modelling and optimization framework

Zhang, R. *et al. Computers & Chemical Engineering*, 2016, 93, 87–100.

Inter-city high-speed passenger transport, mainly aviation and high-speed railway, has been increasing around the world, in accordance with economic development and penetration of high-speed transport technologies. The energy consumption over the lifetime of transport infrastructure and operation is a significant factor at the planning stage. This paper presents a superstructure modelling and optimization framework of inter-city high-speed transport systems, accounting energy consumption during infrastructure construction and during subsequent operation, to optimize connections between large population centres and between modes of transport. Energy consumption during infrastructure construction is obtained from investment cost using lifecycle assessment. The first two cases considered differences between infrastructure construction and lifetime operation while the second case narrowed the study scope. Sensitivity analysis in the third case compared impacts of both transport means on system design. Model results have implications for actual high-speed transport technology development and infrastructure layout.

17/02326 Cool materials for reducing summer energy consumptions in Mediterranean climate: in-lab experiments and numerical analysis of a new coating based on acrylic paint

Antonaia, A. *et al. Applied Thermal Engineering*, 2016, 102, 91–107.

The urbanization has negative effects on the environment, mainly related to the generation of pollution, the modification of the properties of the atmosphere, the covering of the soil surface. The cumulative effects produce the so-called phenomenon of 'urban heat island' (UHI). Cool roofs have a positive impact on the global environment, by reducing the energy required for interior cooling and related greenhouse gas emissions. Moreover these help to mitigate the UHI effect. A cool roofing material is characterized by higher solar reflectance in comparison to conventional roof coatings and high infrared emittance values. This paper is aimed to investigate the potentialities of high reflective commercial products not specialized for cool roofing. Three paints of the automotive sector have been selected. These products have very fast drying, good adhesion directly to different type of materials, good gloss and appearance, greater durability than traditional, lower cost and application time. Laboratory measurements are performed for the characterization of thermal-optical properties of different prototype samples, by considering application on different substrates (aluminium, ceramic tile, bitumen membrane, polyvinyl chloride sheet) as well as different configurations (evaluating the adoption of gripping and external gloss). Only the white acrylic paint shows good values for spectral reflectance (77–80%) and thermal emissivity (92%) that are comparable with commercial products. The artificial accelerated weather resistance tests and natural exposure effects have been also evaluated. Then, several numerical analyses are proposed for a real case study and some roof technologies also with different insulation level. The main evaluated indexes are the seasonal and annual energy savings, the reduction of polluting emissions and the cost effectiveness. Globally summer benefits are very satisfying meanwhile the annual energy saving varies between 0.3% and 3.0%.

17/02327 Cost-benefit analysis of integrating BIPV-T air systems into energy-efficient homes

Delisle, V. and Kummert, M. *Solar Energy*, 2016, 136, 385–400.

The market share of building-integrated photovoltaics (BIPV) remains limited. One of the main barriers to its larger adoption is its initial capital cost, as BIPV is generally more expensive than traditional roof or façade mounted photovoltaic modules (PV). Converting BIPV systems into BIPV with thermal energy recovery (BIPV-T) can improve its benefit and competitiveness compared to other solar energy technologies. This benefit is difficult to estimate, however, as it strongly depends on the usefulness of the thermal energy produced and the incremental cost of the technology to recover the heat. This study aims at evaluating the cost-benefit of BIPV-T focusing on systems that use air as the heat recovery fluid and are integrated into all-electric energy-efficient homes located in heating dominated climates. This cost-benefit is evaluated using the concept of break-even cost defined as the maximum incremental cost to convert a BIPV system into a BIPV-T system to break-even with the cost of (a) a BIPV system and (b) side-by-side PV modules and solar thermal collectors (PV + T). To obtain this cost, the useful equivalent energy production of BIPV, BIPV-T and PV + T systems was first obtained for six energy-efficient housing archetypes located in various cities across Canada. Four different heat management scenarios were considered for the BIPV-T system: (1) fresh air preheating, (2) domestic hot water preheating through an air-to-water heat exchanger, (3) domestic hot water and space heating with an air-to-water heat pump and (4) domestic hot water heating with a heat pump water heater. Compared to BIPV, BIPV-T systems always produce more useful energy and as a result, the break-even cost compared to a BIPV system was found to be always positive and up to C$2700 for a medium two-storey home located in Montreal. For that same house and considering the price of BIPV equal to that of standard roof-mounted PV modules, the break-even cost of a BIPVT system compared to a PV + T system was estimated at C$4200. If the price of BIPV were to get 10% lower than PV, however, this break-even cost could increase to C$6400.

17/02328 Designing optimized energy scenarios for an Italian Alpine valley: the case of Giudicarie Esteriori

Mahbub, M. S. *et al. Energy*, 2016, 116, 236–249.

The design of future local energy scenarios, under the framework of covenant of mayors' initiative, is an important and challenging task for the energy and policy planners. Designing energy scenarios is a multi-objective optimization problem, hence, a framework that combines a multi-objective evolutionary algorithm and EnergyPLAN is employed to identify optimized scenarios. In this study, optimized scenarios for the policy makers of Giudicarie Esteriori are identified, so that they are able to face the challenges of minimizing energy costs and CO_2 emissions, decreasing the dependency on foreign resources, and integrating large amount of renewable energy. The results show that economically attractive, environmental friendly and less dependent energy scenarios can be achieved by (1) increasing the capacity of photovoltaics, (2) maximizing local biomass usage through individual wood boilers and (3) partially electrifying the thermal sector through ground source heat pumps. The modification of the transport sector by introducing electric cars is not economically viable under the current market conditions. This kind of study can be performed for the policy makers of other regions as well, by (1) collecting energy data, (2) identifying local renewable resources, (3) modelling reference scenarios, (4) identifying optimized scenarios and (5) studying the scenarios according to the requirements.

17/02329 Evaluating energy behavior change programs using randomized controlled trials: best practice guidelines for policymakers

Frederiks, E. R. *et al. Energy Research & Social Science*, 2016, 22, 147–164.

Governments and policymakers around the globe are becoming increasingly interested in how to effectively change the behaviour of energy consumers. In the residential sector, numerous programmes are attempting to shift the behaviour of individuals and households in the public interest – for example toward more energy efficient practices, greater uptake of demand-side management technology, increased use of renewable energy, and better responsiveness to new tariffs (e.g. dynamic pricing), to name but a few. However, the effectiveness of such behaviour change interventions is often limited, or even unknown, due to weaknesses in programme design and evaluation of programme impact on behaviour. To help policymakers avoid such pitfalls, this paper outlines some practical guidelines for designing, conducting and, most importantly, evaluating the impact of energy-related behaviour change programmes and initiatives. The authors explain why randomized controlled trials are generally the optimal approach for obtaining scientifically valid estimates of a behavioural programme's efficacy and effectiveness. In parallel, specific guidelines are offered for strengthening the validity, reliability and generalizability of empirical findings about programme impact on behaviour. Adopting these guidelines will help to improve program design and delivery, thereby allowing more accurate evaluation of the true cost-effectiveness, utility and mass-scalability of future energy-related behavioural interventions.

17/02330 Heat pipe structure on heat transfer and energy saving performance of the wall implanted with heat pipes during the heating season

Tan, R. and Zhang, Z. *Applied Thermal Engineering*, 2016, 102, 633–640.

The heat transfer coefficient of the wall implanted with heat pipes (WIHP) is closely related to its energy saving potential. In this paper, the influence factors of heat pipe structure on heat transfer coefficient were analysed to enhance the heat transfer performance of the WIHP, such as the working temperature, the ratio of the evaporating section length (RESL) and the diameter of the heat pipe. The results show that the average equivalent heat transfer coefficient (EHTC) of the WIHP reaches the maximum of 1.24 $W/(m^2 °C)$ at a RESL of 75%, and the RESL should be optimized based on the working-hours-weighted mean temperature. There is an approximately linear relationship between the average EHTC and the diameter of heat pipe. The energy saving potential of a typical building with the WIHP in Tianjin, China was analysed, which shows that the WIHP has a great energy saving potential during the heating season.

17/02331 HEM algorithm based smart controller for home power management system

Rajalingam, S. and Malathi, V. *Energy and Buildings*, 2016, 131, 184–192.

The home power management system is proposed with the objective to reduce the electricity cost and also to avoid the problem of high peak demand. Recently more methods have been discussed in the area of home energy management (HEM), but prioritizing the operation of power units from customer point of view has its own benefits depending on the comfort level. The proposed home consists of a smart electrical appliance, photovoltaic system with battery, smart communication network and a robust controller. This controller schedules the power units in response to electricity price at the time of use (ToU). The available power units comprising of solar power, battery power, grid supply and the utilization of home appliance are categorized and monitored regularly. The Primary power units, preferably solar are chosen automatically as per the priority of the customer. When the primary power unit (solar) is not able to supply power, due to its intermittent nature of generation, the controller shifts to next power units accordingly. The simulation results show that the proposed system based on the HEM algorithm reduces the electricity cost, peak demand problem and enhances the efficiency of energy use. The ToU is considered for reducing the peak demand. The smart controller is operated based on HEM algorithm and selects the power units accordingly. Also, there is a necessity of Energy conversion from DC (solar) to AC (grid/appliance), there is feasibility of power quality disturbance. This quality of power is improved by using the selective harmonic elimination method. The proposed system is developed and simulated in MATLAB/SimPowerSystem.

17/02332 Household analysis identifies water-related energy efficiency opportunities

Kenway, S. J. *et al. Energy and Buildings*, 2016, 131, 21–34.

Water heating accounts for around one-third of household direct energy use. This energy demand is some four times greater than lighting. Here the authors use detailed monitoring and modelling of seven individual households to quantify major factors. Using normalized sensitivity results they demonstrate (i) high variability and (ii) a large and consistent influence of shower duration, flow rate, frequency and temperature along with hot water system efficiency, adult population, and the temperature of cold water. A 10% change in these factors influenced 0.1–0.9 kWh/hh-person-day, equivalent to a 2–3% of total household energy use. The authors draw on 5399 shower events from a further 94 households, and 491 shower temperature measurements to understand the scope for changes to the households. Individual parameters variation guided by these larger datasets demonstrated shower duration and flow rate offer most scope for change. This study helps guide city-scale analysis of household water-related energy demand. It also supports the tailoring of behavioural and technological water-efficiency programs towards those with strongest potential to influence energy. Strong interaction between parameters suggests that programmes aiming to influence water-related energy need to be aware of how this interplay either amplifies, or diminishes, the intended energy savings.

17/02333 On the oversupply of heat to bedrooms during winter in highly insulated dwellings with heat recovery ventilation

Berge, M. *et al. Building and Environment*, 2016, 106, 389–401.

The study presented in this paper originated from observations made regarding the thermal conditions during winter in highly insulated dwellings with mechanical ventilation with heat recovery (MVHR). Previous observations indicate an oversupply of heat to bedrooms and a successive extensive window ventilation, which leads to an increased space-heating demand. Detailed simulations were conducted to explain the causes for the observed thermal conditions and to elaborate improved solutions for heating and ventilation during winter. Various MVHR solutions and control strategies, as well as building design solutions, were investigated regarding their impact on the thermal conditions in bedrooms and on the space-heating demand. The results clearly illustrates that the supply-air temperature and the temperatures in the living room and bathroom have substantial effects on the thermal conditions in the bedrooms. A one-zone MVHR solution, with approximately the same the supply-air temperature to all rooms, has clear limitations regarding the provision of thermal comfort in bedrooms. The clear potential of a two-zone MVHR solution, where the supply-air temperature to the bedrooms is controlled independently from other rooms, was observed. With a two-zone MVHR solution, the thermal conditions in bedrooms can be improved and the space-heating demand can be reduced.

17/02334 Optimising urban energy systems: simultaneous system sizing, operation and district heating network layout

Morvaj, B. *et al. Energy*, 2016, 116, 619–636.

Distributed and decentralized energy systems coupled with district heating networks are promising concepts for achieving less carbon-intensive urban energy systems. This paper investigates the optimal design and operation of distributed energy systems as well as optimal heating network layouts for different economic and environmental objectives. A mixed integer linear programming model was used for multi-objective optimization to minimize total cost and carbon emissions. Improvements include the coupling of equipment and network modelling across many buildings, detailed combined heat and power (CHP) operational constraints, the inclusion of network heat losses, and improved modelling of thermal storage. The model was used on a case study consisting of 11 residential buildings and one commercial building for various design scenarios (available technologies, network layout limitations, operating constraints). Design results (capacities, network layouts) and operational results (energy supply breakdowns) are presented. The results show that district heating can deliver emissions savings of 23% over a standard solution for the same cost. The optimal number of heating network links increases as more stringent carbon emissions targets are implemented. Limits on possible network routes have significant impacts on the optimal technology capacities and on operational schedules. Also, commonly neglected constraints on CHP operation cause noticeably more reliance on district heating networks.

17/02335 Potential for energy savings by heat recovery in an integrated steel supply chain

McBrien, M. *et al. Applied Thermal Engineering*, 2016, 103, 592–606.

Heat recovery plays an important role in energy saving in the supply chain of steel products. Almost all high temperature outputs in the steel industry have their thermal energy exchanged to preheat inputs to the process. Despite the widespread development of heat recovery technologies within process stages (process heat recovery), larger savings may be obtained by using a wider integrated network of heat exchange across various processes along the supply chain (integrated heat recovery). Previous pinch analyses have been applied to optimize integrated heat recovery systems in steel plants, although a comparison between standard process heat recovery and integrated heat recovery has not yet been explored. In this paper, the potential for additional energy savings achieved by using integrated heat recovery is estimated for a typical integrated steel plant, using pinch analysis. Overall, process heat recovery saves approximately 1.8 GJ per tonne of hot rolled steel (GJ/t h), integrated heat recovery with conventional heat exchange could save 2.5 GJ/t h, and an alternative heat exchange that also recovers energy from hot steel could save 3.0 GJ/t h. In developing these networks, general heat recovery strategies are identified that may be applied more widely to all primary steel production to enhance heat recovery. Limited additional savings may be obtained from the integration of the steel supply chain with other industries.

17/02336 Prediction of residential building energy consumption: a neural network approach

Biswas, M. A. R. *et al. Energy*, 2016, 117, 84–92.

Some of the challenges to predict energy utilization has gained recognition in the residential sector due to the significant energy consumption in recent decades. However, the modelling of residential building energy consumption is still underdeveloped for optimal and robust solutions while this research area has become of greater relevance with significant advances in computation and simulation. Such advances include the advent of artificial intelligence research in statistical model development. Artificial neural network has emerged as a key method to address the issue of non-linearity of building energy data and the robust calculation of large and dynamic data. The development and validation of such models on one of the TxAIRE Research houses has been demonstrated in this paper. The TxAIRE houses have been designed to serve as realistic test facilities for demonstrating new technologies. The input variables used from the

house data include number of days, outdoor temperature and solar radiation while the output variables are house and heat pump energy consumption. The models based on Levenberg–Marquardt and OWO–Newton algorithms had promising results of coefficients of determination within 0.87–0.91, which is comparable to prior literature. Further work will be explored to develop a robust model for residential building application.

17/02337 Reflections on retrofits: overcoming barriers to energy efficiency among the fuel poor in the United Kingdom

Fylan, F. *et al. Energy Research & Social Science*, 2016, 21, 190–198.

To meet targets on fuel poverty, energy efficiency and carbon emissions, existing homes need to be more energy efficient. The authors report the results of a participatory action research project to explore the challenges associated with energy efficiency retrofit programmes and ways to better implement future schemes. Six focus groups were held with 48 participants from a range of energy efficiency roles. Data were analysed thematically using the research question 'What are the challenges presented by implementing energy efficiency retrofit programmes?'. Four themes were identified in the data: Funding mechanisms; Predicting performance; Installation and People. Challenges include funding mechanisms for retrofit programmes resulting in insufficient time to plan, publicize, implement and evaluate a scheme and insufficient flexibility to specify the most appropriate intervention for individual homes. Site workers sometimes need to adapt retrofit designs because of insufficient detail from the designer and can equate quality of installation with quality of finish. Landlords and occupier behaviour can impact on the programme's success and there is a need for greater information on benefits for landlords and for energy behaviour change interventions run alongside retrofit programmes for occupiers. There is a need for outcome evaluations of retrofit schemes with the results shared with stakeholders.

17/02338 Replacement or additional purchase: the impact of energy-efficient appliances on household electricity saving under public pressures

Mizobuchi, K. and Takeuchi, K. *Energy Policy*, 2016, 93, 137–148.

This study examined the influence of additional and replacement purchases of energy-efficient air-conditioners on power savings. The authors used a questionnaire survey and measured electricity use data from 339 Japanese households, collected from two city areas with different level of government-requested electricity-saving rates, namely, Osaka (10%) and Matsuyama (5%). The main findings of this study are as follows. (1) Households that purchased energy-efficient air-conditioners saved more electricity than those that did not. (2) 'Additional-purchase households' showed significant energy savings, whereas 'replacement households' did not. The rebound effect may negate the energy-saving effects of a new air-conditioner. (3) Altruistic attitude is associated with more active participation in power saving. (4) Households in Osaka saved more electricity than those in Matsuyama, probably because the government call to save electricity was more forceful.

17/02339 Saving energy is not easy: an impact assessment of Dutch policy to reduce the energy requirements of buildings

Vringer, K. *et al. Energy Policy*, 2016, 93, 23–32.

The Dutch government stimulates the application of energy efficiency measures to reduce the energy requirements of buildings, which are responsible for about 20% of the Dutch CO_2 emissions. For this assessment, a qualitative approach was followed, due to a lack of data. The authors reviewed the mix of policy instruments and used stakeholder surveys and interviews. It was found that energy use is not very likely to decline fast enough to achieve the Dutch policy targets for 2020. For new buildings, the policy mix works well, but its contribution to the policy targets is limited. For non-residential buildings the current Act, which obliges enterprises to take cost-effective measures, could be enforced to a greater degree. For privately owned homes a more compelling policy is needed. An alternative policy option would be to make taxation dependent on the energy label of residential houses. This would stimulate residents to take action while retaining the desired autonomy. For rental housing, binding agreements between municipalities and housing corporations may lead to more energy saving measures. Finally, it was concluded that the Dutch energy tax is an important pillar of the current policy. It provides higher cost-effectiveness of energy saving measures and legitimates more strict energy efficiency standards.

17/02340 Schatzkian practice theory and energy consumption research: time for some philosophical spring cleaning?

Galvin, R. and Sunikka-Blank, M. *Energy Research & Social Science*, 2016, 22, 63–68.

The version of practice theory developed by Theodore Schatzki is employed increasingly in energy consumption research. This emerged in response to problems Wittgenstein had identified in the core logic of prevailing rule-based, inter-subjectivist social theories of the late twentieth century. Since then, however, the use and development of Schatzkian practice theory in energy studies has not been subjected to ongoing, robust philosophical critique. This paper offers some thoughts on how such a critique might proceed. It begins by outlining the roots of Schatzki's version of practice theory in his critique of Giddens and Bourdieu. It then explores three areas where practice theory appears to need more in-depth critique and development: a fuller account of the ontological status of 'practices' and what this implies for research models; more clarity on lines of causality; and the place of socio-economic issues within practices and their descriptions. It concludes that practice theory provides a very insightful framework for heuristic models in energy research but that its usefulness is held back by these yet unresolved difficulties.

17/02341 Strategy for the energy renovation of the housing stock in Comunitat Valenciana (Spain)

Serrano-Lanzarote, B. *et al. Energy and Buildings*, 2016, 132, 117–129.

The Spanish residential building stock built between 1940 and 1980 period presents a high energy saving potential as it represents a significant percentage of the total housing stock and it was built without any regulation regarding energy efficiency. Accordingly, the first aim of this paper was to quantify the energy saving potential and the related reduction in CO_2 emissions of the housing stock in those years. The work focuses on the Mediterranean climate of the Comunitat Valenciana region, therefore the energy efficiency strategies proposed are passive and deal with the envelope of buildings. On the basis of the results obtained, several scenarios with intervention periods of 10, 20 and 30 years were calculated. The conclusion was that with the current rate of annual building renovation, it will be nearly impossible to reach the goals established by the EU's Energy Performance in Buildings Directive. Only a deep transformation of the building fabric within this sector could help in achieving them. Finally, it should be noted that the proposed methodology can be applied to other areas with different climates, particularly in Spain.

17/02342 The energy-saving effects of ground-coupled heat pump system integrated with borehole free cooling: a study in China

Zhou, Z. *et al. Applied Energy*, 2016, 182, 9–19.

Ground coupled heat pump (GCHP) systems have been widely implemented due to its potential benefits of energy savings. However, very few studies attempted to examine the operational performance of GCHP system integrated with borehole free cooling (i.e. using the circulating water in ground heat exchanger for the cooling purpose). A typical office building in Tianjin was chosen for a detailed case study. Both experiments and numerical simulation are employed to examine the efficiency of proposed GCHP system by means of comparing the normal running mode (NRM) and the energy-saving running mode (ESRM) in terms of the energy consumption and soil temperature variation. The results showed that the energy efficiency ratio (EER_{system}) of the system increased every year in winter but decreased gradually in summer during 10 years of operation. In winter, the EER_{system} of NRM was 3.4% higher than that of ESRM. In summer, the EER_{system} of NRM was 0.5% lower than that of ESRM under the same normal cooling mode (NM_c). The EER_{system} of free cooling mode (FM_c) could reach as high as 23.35, which was 5.2 times higher than that of NM_c. In summer, the EER_{system} of ESRM was 13.58 on average, which was 2.6 times higher than that of NRM. The soil temperature gained minor rise under both modes during 10 years of operation. This study revealed that there are significant energy savings benefits if the GCHP system is integrated with FM_c. Meanwhile, the requirements related to temperature and humidity can be satisfied when the indoor thermal and moisture load are not too high. Therefore, the integration of FM_c with GCHP system could be considered for the operation of office buildings in the future.

17/02343 The rebound effect and Schatzki's social theory: reassessing the socio-materiality of energy consumption via a German case study

Galvin, R. and Gubernat, A. *Energy Research & Social Science*, 2016, 22, 183–193.

Rebound effect studies are useful for policy making, as they indicate the extent to which increases in energy efficiency lead to lower energy savings than those predicted by engineering calculations. Existing rebound studies assume energy consumption changes arise from an economically rational response, by consumers, to cheaper energy services. This misses the possibility that energy efficiency increases could have effects on wider society, organization and material-human relationships which lead to increases in energy consumption for reasons other than economic utility. This paper argues that setting rebound studies within a properly worked out social theory would give

a fuller picture of these causal routes. Noting that 'practice theories' drawn from Schatzki are being used increasingly in energy consumption studies, the paper critically expounds Schatzki's development of practice theory and human-material 'arrangements', offering this as a framework for rebound studies. It then uses a small case study, of growth in computer use in a university research cluster, to compare rebound effect results obtained by the traditional approach and the Schatzkian approach. The latter gives rebounds up to 100% higher than the former. The paper recommends that policy take these wider causal determinants into account when estimating likely effects of energy efficiency increases.

17/02344 The relationship between house size and life cycle energy demand: implications for energy efficiency regulations for buildings

Stephan, A. and Crawford, R. H. *Energy*, 2016, 116, 1158–1171.

House size has significantly increased over the recent decades in many countries. Larger houses often have a higher life cycle energy demand due to their increased use of materials and larger area to heat, cool and light. Yet, most energy efficiency regulations for buildings fail to adequately include requirements for addressing the energy demand associated with house size. This study quantifies the effect of house size on life cycle energy demand in order to inform future regulations. It uses a parametric model of a typical detached house in Melbourne, Australia and varies its floor area from 100 to 392 m^2 for four different household sizes. Both initial and recurrent embodied energy requirements are quantified using input-output-based hybrid analysis and operational energy is calculated in primary energy terms over 50 years. Results show that the life cycle energy demand increases at a slower rate compared to house size. Expressing energy efficiency per m^2 therefore favours large houses while these require more energy. Also, embodied energy represents 26–50% across all variations. Building energy efficiency regulations should incorporate embodied energy, correct energy intensity thresholds for house size and use multiple functional units to measure efficiency. These measures may help achieve greater net energy reductions.

17/02345 Using fuzzy multiple criteria decision making approaches for evaluating energy saving technologies and solutions in five star hotels: a new hierarchical framework

Mardani, A. *et al. Energy*, 2016, 117, 131–148.

The purpose of this study is to present a hierarchical framework for evaluating and ranking the important key energy-saving technologies and solutions in the 10 biggest Iranian hotels through integrating fuzzy set theory, as well as qualitative and quantitative approaches. The important key energy factors for the evaluation of energy saving technologies and solutions are gathered through a literature survey. This paper proposes a framework based on the fuzzy Delphi method, fuzzy multiple criteria decision-making, including fuzzy analytic hierarchy process and fuzzy techniques for order performance by similarity to ideal solution. In the fuzzy Delphi method step of the study, 17 key energy factors were selected from among a total of 40 energy factors and categorized into five groups. Fuzzy analytic hierarchy process was used for the ranking of 17 key energy factors, and fuzzy techniques for order performance by similarity to ideal solution employed for ranking of the 10 biggest Iranian hotels in different provinces. The results of this study revealed that the first rank of main groups was equipment efficiency (0.403), system efficiency (0.225) had the second rank, third rank was related to reduction of heating and cooling demands (0.151) and energy management (0.091) and renewable energy (0.083) had the fourth and fifth ranks respectively. In the ranking weights of 17 sub-groups of energy saving technologies and solutions, the results of fuzzy analytic hierarchy process showed that efficient solutions for active space cooling (0.662) was as first rank, building insulation had the second rank with score (0.541) and third rank was European Eco-label for tourist accommodation service (0.532).

17/02346 Who exhibits more energy-saving behavior in direct and indirect ways in china? The role of psychological factors and socio-demographics

Yang, S. *et al. Energy Policy*, 2016, 93, 196–205.

This research explores the possibilities for further energy saving in households in the Chinese context by conducting of a survey on energy curtailment behaviours. The study examines how people's demographic characteristics and psychological factors affect their direct and indirect energy curtailment behaviours at home, as well as the different effects of these antecedents. Results suggest that people with high sense of environmental responsibility and curtailment attitude are more likely to engage in both direct and indirect energy curtailment actions. Generally, indirect energy curtailment behaviour is more strongly related to psychological and socio-demographic factors than direct behaviour, and these socio-demographic factors vary for direct and indirect behaviours. Interesting patterns emerged with respect to gender, age, family structure, family income, and level of education. Results indicate that strengthening publicity and education to increase environmental awareness among Chinese urban residents would be effective in reducing household energy consumption, especially when the said measures target a specific population and specific behaviours.

17 ENERGY CONVERSION AND RECYCLING

17/02347 An experimental setup for the analysis of an energy recovery system from wastewater for heat pumps in civil buildings

Postrioti, L. *et al. Applied Thermal Engineering*, 2016, 102, 961–971.

Despite its low enthalpy content, sewage water from civil buildings could represent an interesting source for energy saving, especially when heating and cooling is supplied by heat pumps. A complete prototype plant was realized to assess the characteristics and performance of heat recovery from civil wastewater, used as ancillary thermal supply to a heat pump heating system; during the experimental analysis, the wastewater discharge cycles estimated from data derived by the most common buildings typologies were applied. The warm water fluids were collected in a purposely-built tank-heat exchanger, which represents the thermal storage aimed at improving the heat pump performance. A dedicated software was created to manage the acquisition of thermal fluid dynamic variables of all hydraulic circuits. Results highlighted the potential of a plant performance enhancement in winter conditions, respect to the common solutions with external air–water heat exchangers, once a correct control system is implemented, needed to automate the decision process of sending the water to be heated to the tank or to the external air–water heat exchanger. The heat pump working conditions could even become close to be independent from external air conditions, if the average wastewater input results high enough during the day. The additional cost of the energy recovery system resulted affordable, achieving a reasonable payback period.

17/02348 Biochemical compositions and fatty acid profiles in four species of microalgae cultivated on household sewage and agro-industrial residues

Calixto, C. D. *et al. Bioresource Technology*, 2016, 221, 438–446.

The potential of four regional microalgae species was evaluated in relation to their cell growth and biomass production when cultured in the following alternative media: bio-composts of fruit/horticultural wastes (HB), sugarcane waste and vinasse (VB) chicken excrements (BCE), raw chicken manure (RCM), and municipal domestic sewage (MDS). The cultures were maintained under controlled conditions and their growth responses, productivities, biochemical compositions, and the ester profiles of their biomasses were compared to the results obtained in the synthetic media. The MDS and HB media demonstrated promising results for cultivation, especially of *Chlorella* sp., *Chlamydomonas* sp. and *Lagerheimia longiseta*, which demonstrated productivities superior to those seen when grown on the control media. The highest lipid levels were obtained with the HB medium. The data obtained demonstrated the viability of cultivating microalgae and producing biomass in alternative media prepared from MDS and HB effluents to produce biodiesel.

17/02349 Cascade thermochemical storage with internal condensation heat recovery for better energy and exergy efficiencies

N'Tsoukpoe, K. E. *et al. Applied Energy*, 2016, 181, 562–574.

Thermochemical heat storage processes generally involve significant condensation heat rejection to the environment during charging. This heat rejection is about two-thirds of the charging heat of salt hydrates, which are a promising class of materials for heat storage in the low temperature range, i.e. for space heating and domestic hot water production. This study shows that internal condensation heat recovery through a new concept of a cascade thermochemical heat storage process leads to an improvement of the energy and exergy efficiencies of the process. To illustrate the potential of this new concept, the authors compare a classical thermochemical based heat storage with one involving internal condensation heat recovery. In order to have an unbiased comparison basis, the two processes have similar boundary temperature conditions. The energy and exergy efficiencies of the process with internal heat recovery is as much as 1.8 times that of the classical thermochemical heat storage process. The process with heat recovery requires only 55% of the energy input at high temperature during charging of the classical process, for the same discharging heat output.

17/02350 Characterizing the performance of a single-screw expander in a small-scale organic Rankine cycle for waste heat recovery

Ziviani, D. *et al. Applied Energy*, 2016, 181, 155–170.

This paper focuses on the experimental and numerical characterizations of a single-screw expander for waste heat recovery organic Rankine cycle (ORC) applications. A down-scaled industrial ORC test-rig has been tested with two different working fluids, R245fa and SES36. The hot source inlet temperature has been set to 125 °C and the maximum expander inlet pressure was limited to 1200 kPa. A total of 102 steady-state points have been collected by varying the expander pressure ratio between 3 and 9 with rotational speeds in the range from 2000 to 3300 rpm. The experimental results allowed to assess the relationship between internal built-in volume ratio and imposed expansion ratio at different rotational speeds with respect to shaft and overall isentropic efficiency as well as volumetric performance in terms of filling factor. Results showed that while R245fa allowed approximately a 10% higher power output, the single-screw expander was performing at higher isentropic efficiency with SES36 due to higher pressure ratio achievable under the given working conditions and system limitations which also led to a better matching between ORC system and volumetric expander performance. A semi-empirical model has been developed and calibrated to break down the expander internal losses in the case of R245fa. The model has been exercised to investigate the effect of potential design improvements on the overall performance. The friction losses played a major role in the total loss count followed by suction pressure drops and leakages. As a consequence, the effect of lubrication should be further investigated to reduce leakages and friction. This study demonstrates the potential of single-screw technology as volumetric expander for ORC applications.

17/02351 Continuous treatment of high strength wastewaters using air-cathode microbial fuel cells

Kim, K.-Y. *et al. Bioresource Technology*, 2016, 221, 96–101.

Treatment of low strength wastewaters using microbial fuel cells (MFCs) has been effective at hydraulic retention times (HRTs) similar to aerobic processes, but treatment of high strength wastewaters can require longer HRTs. The use of two air-cathode MFCs hydraulically connected in series was examined to continuously treat high strength swine wastewater (7–8 g/L of chemical oxygen demand, COD) at an HRT of 16.7 h. The maximum power density of $750 \pm 70\,mW/m^2$ was produced after 12 days of operation. However, power decreased by 85% after 185 days of operation due to serious cathode fouling. COD removal was improved by using a lower external resistance, and COD removal rates were substantially higher than those previously reported for a low strength wastewater. However, removal rates were inconsistent with first order kinetics as the calculated rate constant was an order of magnitude lower than rate constant for the low strength wastewater.

17/02352 Drain water heat recovery storage-type unit for residential housing

Torras, S. *et al. Applied Thermal Engineering*, 2016, 103, 670–683.

The drain water heat recovery (DWHR) system is an interesting household technology to reduce energy costs and environmental impact. The objective of the utilization of these devices is the recovery of the waste heat from domestic warm drain water, and transferring it to cold water entering the house. A drain water heat recovery unit has been built in this work. The authors are using both numerical and experimental tools to design and study the performance of this device, focusing on the analysis of a specific drain water heat recovery storage-type based on a cylindrical tank with an internal coiled pipe. The numerical simulation has been performed using an in-house platform, where the different elements of the DWHR storage are linked to solve the system. On the other hand, an experimental infrastructure has been developed to analyse of the system, which has been instrumented to provide detailed information of its heat recovery and storage capacities and temperature map. Different internal flow rates and operational temperatures have been studied. From the results obtained it can be said that the device shows interesting heat recovery and storage capacities, while the numerical platform shows promising comparison results against the experiments.

17/02353 Experimental investigations on a cascaded steam-/organic-Rankine-cycle (RC/ORC) system for waste heat recovery (WHR) from diesel engine

Yu, G. *et al. Energy Conversion and Management*, 2016, 129, 43–51.

A novel cascaded RC/ORC system that comprises a steam Rankine cycle as the high-temperature loop (H-RC) and an organic Rankine cycle as the low-temperature loop (L-ORC) was constructed and experimentally investigated to recover waste heat from exhaust gas of a heavy-duty diesel engine (DE). By monitoring key parameters of the RC/ORC system against time, good system stability and satisfying thermal states of working fluids were observed. Impacts that the engine operations have on this proposed waste-heat-recovery (WHR) system were studied, indicating that waste heat recovered from the gas increases gradually and greatly as the engine load increases, yet decreases slightly as the speed grows. At full loads at speeds lower than 2050 rpm, up to 101.5 kW of waste heat can be abstracted from the gas source, showing a promising heat transfer potential. Besides, observations of key exergy states as well as estimations and comparisons of potential output power were carried out stepwise. Results indicated that up to 12.7 kW of output power could be obtained by the novel RC/ORC system under practical estimations. Comparing to the basic diesel engine, the power increment reaches up to 5.6% by equipping the cascaded RC/ORC system.

17/02354 High-methane gasification of fuels from waste – experimental identification

Król, D. and Poskrobko, S. *Energy*, 2016, 116, 592–600.

The paper presents experimental research on innovative technology of refused derived fuel (RDF) produced from combustible waste (other than hazardous) gasification. The gasification process was performed in the compact bed, in the laboratory tubular gas generator with a power of 5 kW. In the first place RDF, not enriched with methane, was gasified with addition of Bio-CONOx. Next, cogasification was performed with 10%, 15% and 20% addition of methane-forming formulation. The results indicated that the addition of Bio-CONOx to the fuel resulted in an increase in the content of CH_4 in the syngas (8% without the addition of Bio-CONOx to 18% CH_4 with a 20% addition of Bio-CONOx). At the same time there was an increase in shares of other combustible components of syngas (CO and H_2). Enriching fuel with the additive Bio-CONOx increased the calorific value of the syngas LHV from $4\,MJ/N\,m^3$ (RDF) to $9\,MJ/N\,m^3$ (RDF with 20% addition of Bio-CONOx). Studies have shown that the increase in efficiency of the gasification process has been obtained by setting the process conditions in a tubular reactor, i.e. temperature decomposition: 400–450 °C in the layer of fuel and 800–850 °C in the gas zone above the layer of fuel. Such temperature distribution in the layer of fuel favours exothermic process of hydrogenation of CO and CO_2 to CH_4 form and evaporation and decomposition of fat fraction contained in methane forming supplement. At high temperatures over a layer of fuel (in the atmosphere of unreacted oxygen), some organic vapours (greases and tars) were burnt, and some underwent cracking.

17/02355 Hybrid model for heat recovery heat pipe system in liquid desiccant dehumidification system

Shen, S. *et al. Applied Energy*, 2016, 182, 383–393.

In this paper, a hybrid model for heat pipe heat exchanger used for heat recovery in regenerator of the liquid desiccant dehumidification system (LDDS) is developed. The proposed hybrid model starts from the physical governing equations and lumps the complex geometric parameters and fluids' thermodynamic coefficients as constants since they have very small changes during the process operation. The resulting model has only three unknown parameters which can be determined by Levenberg–Marquardt method. Compared with the existing heat pipe models, the proposed model is very simple, accurate, and does not require iterative computations. A large amount of testing for the heat pipe heat exchanger installed in a pilot LDDS shows that the model is very effective to predict the performance in a wide operating range. The model is expected to find its applications in monitoring, control and optimization of the regenerator heat recovery process of LDDS.

17/02356 Kinetics of coffee industrial residue pyrolysis using distributed activation energy model and components separation of bio-oil by sequencing temperature-raising pyrolysis

Chen, N. *et al. Bioresource Technology*, 2016, 221, 534–540.

This study was carried out to investigate the kinetics of coffee industrial residue (CIR) pyrolysis, the effect of pyrolysis factors on yield of bio-oil component and components separation of bio-oil. The kinetics of CIR pyrolysis was analysed using distributed activation energy model, based on the experiments in thermogravimetric analyser, and it indicated that the average of activation energy (E) is $187.86\,kJ \cdot mol^{-1}$. −1. The bio-oils were prepared from CIR pyrolysis in vacuum tube furnace, and its components were determined by gas chromatography/mass spectrometry. Among pyrolysis factors, pyrolysis temperature is the most influential factor on components yield of bio-oil, directly concerned with the volatilization and yield of components (palmitic acid, linoleic acid, oleic acid, octadecanoic acid and caffeine). Furthermore, a new method (sequencing temperature-raising pyrolysis) was put forward and applied to the components separation of bio-oil. Based on experiments, a solution of components separation of bio-oil was come out.

17/02357 Simultaneous microalgal biomass production and CO_2 fixation by cultivating *Chlorella* sp. GD with aquaculture wastewater and boiler flue gas

Kuo, C.-M. *et al. Bioresource Technology*, 2016, 221, 241–250.

A microalgal strain, *Chlorella* sp. GD, cultivated in aquaculture wastewater (AW) aerated with boiler flue gas, was investigated. When AW from a grouper fish farm was supplemented with additional nutrients, the microalgal biomass productivity after 7 days of culture was $0.794\,g\,L^{-1}\,d^{-1}$. CO_2 fixation efficiencies of the microalgal strains aerated with 0.05, 0.1, 0.2 and 0.3 vvm of boiler flue gas (containing approximately 8% CO_2) were 53, 51, 38 and 30%, respectively. When the microalgal strain was cultured with boiler flue gas in nutrient-added AW, biomass productivity increased to $0.892\,g\,L^{-1}\,d^{-1}$. In semi-continuous cultures, average biomass productivities of the microalgal strain in 2-, 3- and 4-day replacement cultures were 1.296, 0.985, and $0.944\,g\,L^{-1}\,d^{-1}$, respectively. These results demonstrate the potential of using *Chlorella* sp. GD cultivations in AW aerated with boiler flue gas for reusing water resources, reducing CO_2 emission, and producing microalgal biomass.

17/02358 Technical and economic analyses of waste heat energy recovery from internal combustion engines by the organic Rankine cycle

de Oliveira Neto, R. *et al*. *Energy Conversion and Management*, 2016, 129, 168–179.

Due to its low complexity, the organic Rankine cycle (ORC) can be considered as one of the best options for waste heat recovery at low (at most 230 °C) and average (230–650 °C) temperatures. A technical and economic study has been conducted in this work in order to increase the efficiency of electricity production, and thus reduce fuel consumption and polluting gas emission from internal combustion engines (ICEs). For such a purpose, two ORC sets were suggested. The first one is facing deployment in water shortage areas (ORC using a cooling tower for the condensing system) and another one with the water supply condenser being made by the urban water net. Both simulated systems were able to increase electricity production by almost 20% when toluene was the working fluid. The economic analysis was based on the engineering chemical cost plant index model which showed that the financial return from the implementation of the ORC system can occur in six years. Thus, it is noted that the ORC system can be installed in areas where there is no water abundance and without much yield loss. Despite being an appropriate technological solution to recover the waste heat present in ICEs' exhaust gas, it still lacks in governmental incentives for a wide application of the system.

17/02359 Upgrading of mesophilic anaerobic digestion of waste activated sludge by thermophilic pre-fermentation and recycle: process performance and microbial community analysis

Wu, L.-J. *et al*. *Fuel*, 2016, 169, 7–14.

In order to upgrade the conventional mesophilic anaerobic (MD) of waste activated sludge (WAS), a thermophilic pre-fermentation and a recycle system were introduced to form continuous thermophilic–mesophilic temperature-phased anaerobic digestion (TPAD) and TPAD with recycling capability (TPAD-R). The synchronous operation, with the MD as control, indicated significant improvements in reduction of solids and the ability to produce methane in the TPAD and TPAD-R, with a similar amount of improvement in both systems. VS reduction was improved from about 40% in the MD to 50%, and the methane recovery rates were improved from 0.53 L/g VS destroyed in the MD to 0.63 L/g VS destroyed accordingly. The thermophilic stage in the TPAD and TPAD-R made a large contribution to organic matter degradation and solubilization, and the specific hydrolysis rate in thermophilic stage attained 0.2 gCOD/g VS/d. Furthermore, under experimental conditions, the thermophilic stage in the TPAD and TPAD-R also played an important role in acidogenesis and methanogenesis. The thermophilic pre-fermentation made *Firmicutes* and *Methanosarcina* become the main phylum and genus in the mesophilic stage, accounting for 44% and 54%, respectively. The recycle system improved the diversity of bacteria and archaea in the thermophilic stage of the TPAD-R. The TPAD and TPAD-R also achieved about twice the net energy of the MD.