01 SOLID FUELS

Sources, winning, properties

14/01833 Characterization of the stress sensitivity of pores for different rank coals by nuclear magnetic resonance

Li, S. *et al. Fuel*, 2013, 111, 746–754.

Nuclear magnetic resonance (NMR) experiments of stress sensitivity on the pore and fracture systems of coal samples with different ranks were performed. Pore compressibility was calculated based on the NMR results. The relationship between pore compressibility and effective stress was discussed and a mathematical model for pore compressibility was developed to describe the experimental data. The experimental results showed different characteristics of NMR T_2 distributions, which were in good accordance to the diverse pore and fracture structures for the different rank coals. Medium and high rank coals have more developed pore space for adsorption, and the main peak of T_2 spectra locate at the low T_2 value section; while for the low rank coals, all the pores and fractures are well developed, with peaks corresponding to them are all obvious on the T_2 spectra. Furthermore, the pore spaces showed different stress sensitivity for different rank coals. For low rank coals, seepage space changes dramatically as the confining pressure changes, and seepage space is the main controlling factor of stress sensitivity. As the metamorphism degree increasing, adsorption space becomes dominant in the pore and fracture structure of coals. Thus adsorption space in high and medium rank coals decreases significantly with the increase of the confining pressure, and stress sensitivity is controlled by their adsorption space, as suggested by the experimental results. The pore compressibility of the coals decreases with confining pressure increase and the experimental data can be accurately described by the newly developed stress-dependent pore compressibility model.

14/01834 Comparison of staged combustion properties between bituminous coals and a low-rank coal; fiber-shaped crystallized carbon formation, NO_x emission and coal burnout properties at very high temperature

Taniguchi, M. *et al. Combustion and Flame*, 2013, 160, (10), 2221–2230.

The authors previously have developed a new-concept for a drop-tube furnace in order to investigate staged combustion properties for pulverized coals. Two high-temperature electric furnaces were connected in series. Coal was burnt under fuel-rich conditions in the first furnace, then, staged air was supplied at the connection between the two furnaces. In the present study, the authors investigated influence of burning temperature on NO_x emission and combustion efficiency by using the furnace. The influence of the temperature differed between hv-bituminous coals and a sub-bituminous coal. For the hv-bituminous coals, combustion efficiency was improved when burning temperature in the fuel-rich region rose. When combustion efficiency was improved, NO_x emission decreased. The NO_x reduction reaction in the fuel-rich region was promoted by increasing the burning temperature in this region. On the other hand, NO_x emission increased for the sub-bituminous coal when the temperature was higher than 1800 K. Usually, combustion efficiency was increased with burning temperature. However, combustion efficiency lowered for the sub-bituminous coal when burning temperature was higher than 1900 K. It was observed the ash obtained by this temperature condition using scanning electron microscopy and transmission electron microscopy and observed fibre-shaped carbon. The difference in NO_x properties was derived as a difference of hydrocarbon concentration. For low-rank coals (sub-bituminous or lignite), the hydrocarbon formation rate was smaller than that for hv-bituminous coals. When the hydrocarbon contribution to the NO_x reduction reaction was large, NO_x emission decreased with increasing burning temperature; however, hydrocarbon content in volatile matter was small for low-rank coals.

14/01835 Factors controlling geochemical and mineralogical compositions of coals preserved within marine carbonate successions: a case study from the Heshan coalfield, southern China

Dai, S. *et al. International Journal of Coal Geology*, 2013, 109–110, 77–100.

The Late Permian coals in the Heshan coalfield of southern China are preserved within marine carbonate successions and characterized by super-high organic sulfur (5.13–10.82%). Minerals identified in the coals include quartz, kaolinite, illite, mixed layer illite/smectite, albite, pyrite, marcasite, calcite, and dolomite, along with trace amounts of smectite, fluorite, strontianite, REY-bearing carbonate minerals, jarosite, and water-bearing Fe-oxysulfate. The coals are very rich in trace elements including F (up to 3362 μg/g), V (up to 270 μg/g), Se (up to 24.4 μg/g), Mo (up to 142 μg/g), U (up to 111 μg/g), and, to a lesser extent, Sr, Y, Zr, Nb, Cd, Cs, heavy rare earth elements, Hf, Ta, W, Hg and Th. Previous studies attributed the high organic sulfur and elevated trace elements to the seawater influence or the formation of soil horizons before the accumulation of peat in the basin. However, mineralogical and geochemical data presented in this study have shown that the sediment-source region and multi-stage hydrothermal fluids are the dominant influences on the mineralogical composition and elevated trace elements in the coal, although seawater influence also contributed to the composition of the mineral matter. For example, a large proportion of the quartz and clay minerals, as well as almost all the albite, in both the coal benches and the parting mudstones were derived from detrital materials of terrigenous origin in the Yunkai Upland. High concentrations of lithophile trace elements were also derived from the sediment source region. Minerals including fluorite, calcite, dolomite, strontianite, and REY-bearing carbonate minerals were derived from multi-stage hydrothermal activities. High concentrations of V, Mo and U that occur through the coal seam sections were probably derived from hydrothermal solutions during peat accumulation or at the early diagenetic stages. The hydrothermal fluids also corroded the syngenetically-formed minerals (quartz, albite and pyrite) and caused redistribution of lithophile elements from partings to the underlying coal benches, resulting in higher key element ratios (Yb/La, Nb/Ta and Zr/Hf) and more abundant heavy rare earth elements in the coal benches than in the immediately overlying partings.

14/01836 High-resolution three-dimensional imaging of coal using microfocus X-ray computed tomography, with special reference to modes of mineral occurrence

Golab, A. *et al. International Journal of Coal Geology*, 2013, 113, 97–108.

Samples of coal from the Sydney and Bowen basins of eastern Australia have been imaged at high resolution using a large-field, three-dimensional microfocus X-ray computed tomography (μCT) system, with special but not exclusive attention to evaluating the modes of occurrence of the mineral matter within the coal. The samples imaged were 110, 25, 19, 10 and 4 mm in size, yielding voxel dimensions of 54, 30, 12, 6 and 3 μm, respectively. Data collection was carried out using a helical stage, providing images with $>2000^2$ voxels in the horizontal (X–Y) plane and up to 3500 voxels high. Three-dimensional image blocks derived from the scans were examined as cross-sections along orthogonal planes and as perspective images, manipulated to be viewed from any angle. Imaging after saturating the coal with X-ray attenuating brine was also carried out to highlight the distribution of connected micro-pores and cleats, and improve the detail of features seen within the samples. Features evaluated within the coals included the size and three-dimensional distribution of siderite nodules, and different types of mineral infillings in petrifactions of maceral components. Individual macerals could also be identified within the coal, based partly on X-ray density and partly on the associated porosity and structure. In some cases high-resolution images enabled the nature of individual plant particles to be identified within the coal samples. Mineral-filled cleats and open fractures were also evaluated, including the origin of radiating fracture patterns around siderite nodules in vitrinite. In some cases several generations of cleat and/or fractures could be distinguished, and the sequence of their formation and infilling was interpreted. Complementary analyses of the mineral matter in the samples were carried out using X-ray diffraction, as well as examination of polished sections by optical microscopy examination. Images obtained from the μCT scans were also registered against SEM–EDX and QemSCAN images of polished sections prepared from the same samples after scanning, providing a more definitive basis for identifying the different components and for integrating μCT data with results from other petrographic and electron microscope studies.

14/01837 Relationship between random reflectance of ulminite B/collotelinite and technological parameters of Polish low-rank coal

Bielowicz, B. *Fuel*, 2013, 111, 229–238.

The main objective of the study is to determine the correlation between random reflectance of ulminite B/collotelinite and chemical and technological parameters in Polish low-rank coals. The study includes results from 284 samples of humic low-rank coal from Polish deposits tested by the author and supplemented with data from the literature. Research on the properties of different types of coal include: technical analysis, physicochemical and petrographic analysis. Among the studied deposits, the average random reflectance is 0.28, with a standard deviation of 0.06 and the coefficient of variation at 20%. Gross calorific value in the tested coal varies from 7.25 to 26.30 MJ/kg, with average value of 12.46 MJ/kg. Average total moisture in Polish low-rank coal deposits is 47.8% and ranges from 15% up to 60%. Carbon content in the tested coal recalculated to dry ash-free basis varies from 56.4% to 79.0% while on average it is 68.1%. Basic parameters of Polish low-rank coal are characterized by low variability,

while gross calorific value and carbon content are of very low variability. The highest variability is observed in case of ash content and sulfur content. The correlation between random reflectance, gross calorific value and carbon content is very high. There is high correlation between moisture, net calorific value and random reflectance. The analysis shows that it is possible to calculate random reflectance of ulminite B/collotelinite from gross calorific value, carbon content and total moisture with a correlation coefficient equal to 0.97. By analysing the correlation between the measures of the degree of coalification and using multiple regression, it has been found that the suborder of Polish lignite can be determined with use of the random reflectance of ulminite B/collotelinite. Based on the results of multiple regression, it is proposed that the boundary between low-rank C (soft brown coal) and low-rank B (dull brown coal) for Polish low-rank coal should be set at a random reflectance of ulminite B equal to 0.35%.

14/01838 Sample weighted variograms on the sequential indicator simulation of coal deposits

de Souza, L. E. and Costa, J. F. C. L. *International Journal of Coal Geology*, 2013, 112, 154–163.

The variogram is an important function in geostatistical applications such as kriging and various conditional simulation methods. In general, the actual variogram function is unknown for a particular application, and inferred from the experimental data. In the same way as first-order statistics, the experimental variogram is also affected by preferentially clustered data. The irregularity of sampling has a well-known destructuring effect on the sample variograms, but it is rarely considered in their experimental calculation and modelling. This paper presents a study where a declustering method based on the data polygon of influence was applied in order to weight data pairs in experimental variogram calculations. The sample weighted variograms were appropriately modelled and used in sequential indicator simulations of coal thickness in a large Brazilian deposit.

Preparation

14/01839 Application of efficient methods of conditional simulation for optimising coal blending strategies in large continuous open pit mining operations

Benndorf, J. *International Journal of Coal Geology*, 2013, 112, 141–153.

The delivery of in-spec coal qualities is essential for an efficient and environmental friendly operation of modern coal-fired power plants. The design of the mining operation systems and blending opportunities plays a key role in homogenizing variability and improving the prediction of key quality parameters, such as the calorific value. Modern methods of conditional simulation in geostatistics allow for generating several realizations for large deposits capturing *in situ* variability of key quality parameters. Integrating simulated realizations of the deposit with a simulation of transport and blending models of mining operation leads to valuable insights into its performance as a function of the technical design and operational mode. The contribution first reviews the method of generalized sequential Gaussian simulation (GSGS), which is especially designed for computational efficient simulation of large deposits. In a second step, GSGS is applied to a large coal field in eastern Europe. The practical simulation process is described and applied in a complex geological environment of highly variable seam geometry and quality including multiple split seams. Results are applied to a large open pit coal operation to investigate the variability of the calorific value and its behaviour along the extraction, transportation and blending process in a continuous mining environment. The described approach provides a valuable view into the performance of a continuous mining system in terms of homogenization. Conclusions can be drawn to optimize the design of key equipment and to adjust the operation mode to ensure that the customer's requirements in terms of coal quality variability are met with high probability.

14/01840 Co-firing in coal power plants and its impact on biomass feedstock availability

Dumortier, J. *Energy Policy*, 2013, 60, 396–405.

Several US states have a renewable portfolio standard (RPS) and allow for biomass co-firing to meet the RPS requirements. In addition, a federal renewable fuel standard mandates an increase in cellulosic ethanol production over the next decade. This paper quantifies the effects on local biomass supply and demand of different co-firing policies imposed on 398 existing coal-fired power plants. The model indicates which counties are most likely to be able to sustain cellulosic ethanol plants in addition to co-firing electric utilities. The simulation incorporates the county-level biomass market of corn stover, wheat straw, switchgrass and forest residues as well as endogenous crop prices. The scenarios indicate that there is sufficient feedstock availability in southern Minnesota, Iowa, and central Illinois. Significant supply shortages are observed in eastern Ohio, western Pennsylvania, and the tri-state area of Illinois, Indiana and Kentucky which are characterized by a high density of coal-fired power plants with high energy output.

14/01841 Formation of $(Fe_xMn_{2-x})O_3$ solid solution and high sulfur capacity properties of Mn-based/M41 sorbents for hot coal gas desulfurization

Zhang, Y. *et al. Journal of Hazardous Materials*, 2013, 248–249, 81–88.

Several MCM-41 materials were synthesized at different conditions by hydrothermal procedure using cheap and easily available industrial water glass as silica source. Fe doped manganese-based oxide/MCM-41 sorbents were prepared by a sol–gel method. The effects of loadings of metal oxide, Fe/Mn molar ratios over MCM-41 and reaction temperature on the performance of sorbent for hot coal gas desulfurization were investigated. Various techniques such as Brunauer–Emmett–Teller, X-ray diffraction, X-ray photoelectron spectroscopy, laser Raman spectroscopy and high-resolution transmission electron microscopy were used to characterize the sorbents. The result indicated Fe^{3+} ions could occupy a position of Mn^{3+} in cubic lattice of Mn_2O_3 and the $(Fe_xMn_{2-x})O_3$ solid solution is mainly active phase of sorbent. Moreover, the result of nine successive sulfurization–regeneration cycles of sorbent showed high sulfur adsorption capacity and endurable stability of $FeMn_4O_x$/MCM-41 for H_2S removal.

14/01842 Oxidation of Shengli lignite with aqueous sodium hypochlorite promoted by pretreatment with aqueous hydrogen peroxide

Liu, F.-J. *et al. Fuel*, 2013, 111, 211–215.

Shengli lignite (SL) was pretreated in H_2O_2 aqueous solution at 40 °C for 4 h to obtain pretreated SL (PTSL). Both the SL and PTSL were oxidized in NaOCl aqueous solution at 30 °C for 5 h to investigate the effect of pretreatment (PT) on SL oxidation with NaOCl. Gas chromatography/mass spectrometry analysis shows that the PT with H_2O_2 significantly increased the yields of alkanoic acids, alkanedioic acids, and benzene carboxylic acids (BCAs), but substantially suppressed the formation of chloro-substituted alkanoic acids (CSAAs). The total yield (daf) of BCAs was 7.4% from SL and increased to 10.1% from PTSL, while that of CSAAs decreased from 5.4% for SL to 0.8% for PTSL. Direct analysis in real time ionization source coupled to mass spectrometry analysis exhibits that the PT with H_2O_2 enhanced the formation of compounds with molecular from m/z 300 to 500. The possible mechanisms for the PT and subsequent oxidation are discussed according to the experimental results. The cleavage of covalent bonds and introduction of oxygen functional groups such as –COOH and –OH by the PT could be responsible for the increase in the yields of soluble species.

Transport, storage

14/01843 An improved relative permeability model for coal reservoirs

Chen, D. *et al. International Journal of Coal Geology*, 2013, 109–110, 45–57.

In this work, the conventional relative permeability model for two-phase flow in porous media is improved to describe the relative permeability for coal. The fracture geometry is considered through applying the matchstick model, instead of the bundle of capillary tubes model which is often used as the conceptual model for conventional porous media, to derive the relative permeability model. The effect of porosity change on relative permeability for coal is taken into account by introducing a residual phase saturation model and a shape factor as functions of permeability ratio. In the improved model, the relative permeability is dependent on both the phase saturation and the porosity (or permeability) change. This improved model shows a strong capability to match the experimental data for different coal relative permeability measurements. Furthermore, the authors evaluate the relative permeability models as a unary function of wetting phase saturation and as a binary function of wetting phase saturation and permeability ratio in a coupled numerical model for water–gas flow in coal seams. The results illustrate that the relative permeability change due to the porosity change can significantly affect the evolution of wetting phase saturation and the gas production rate.

Economics, business, marketing, policy

14/01844 Coal resources, reserves and peak coal production in the United States

Milici, R. C. *et al. International Journal of Coal Geology*, 2013, 113, 109–115.

In spite of its large endowment of coal resources, recent studies have indicated that US coal production is destined to reach a maximum and begin an irreversible decline sometime during the middle of the current century. However, studies and assessments illustrating coal reserve data essential for making accurate forecasts of US coal production have not been compiled on a national basis. As a result, there is a great deal of uncertainty in the accuracy of the production forecasts. A very large percentage of the coal mined in the USA comes from a few large-scale mines (mega-mines) in the Powder River Basin of Wyoming and Montana. Reported reserves at these mines do not account for future potential reserves or for future development of technology that may make coal classified currently as resources into reserves in the future. In order to maintain US coal production at or near current levels for an extended period of time, existing mines will eventually have to increase their recoverable reserves and/or new large-scale mines will have to be opened elsewhere. Accordingly, in order to facilitate energy planning for the USA, this paper suggests that probabilistic assessments of the remaining coal reserves in the country would improve long-range forecasts of coal production. As it is in US coal assessment projects currently being conducted, a major priority of probabilistic assessments would be to identify the numbers and sizes of remaining large blocks of coal capable of supporting large-scale mining operations for extended periods of time and to conduct economic evaluations of those resources.

14/01845 Economic analysis under uncertainty of coal fired capture-ready power plants

Rochedo, P. R. R. and Szklo, A. *International Journal of Greenhouse Gas Control*, 2013, 12, 44–55.

This study assesses the feasibility of investing in capture ready (CR) coal-based power plants under uncertainty. It defines 18 cases according to three routes for carbon capture (post-, pre- and oxy-combustion) and different levels of readiness. Due to the uncertain nature of the development of capture plants, this study applies a probabilistic analysis. Findings for the more likely scenario (median value) indicated that severe pre-investments in CR plants are the best choice only when the implementation of the capture occurs in the short term. In the long term, the investment decision favoured the power plants not fully ready. Interestingly, under a less likely but possible scenario (the inferior limit of the probabilistic analysis) IGCC-ready plants become the best option in the short term, and then oxy-combustion ready plants stand out. Hence, some policies such as those based on financing lowering the discount rate perceived by investors, and those based on fund to research and development, might create an investment environment favourable to CR plants.

14/01846 Engineering and optimization approaches to enhance the thermal efficiency of coal electricity generation in China

Xu, Y. *et al. Energy Policy*, 2013, 60, 356–363.

China has made improving the thermal efficiencies of its coal-fired power plants a national priority. Official data show that the average thermal efficiency was enhanced from 31.3% in 2000 to 33.2% in 2005 and 36.9% in 2010. This paper aims to assess the validity of China's claimed improvement, examine major responsible factors, and identify future improvement opportunities. Recognizable factors can account for about 80% of the reported progress in the tenth Five-Year Plan (2001–2005) and about 85% in the eleventh (2006–2010) to largely verify the reported progress. Engineering approaches – especially replacing inefficient power units with more efficient ones – are the largest contributing factors, while optimization approaches – particularly electricity dispatch – remains inefficient in China. In 2010, the explainable efficiency improvement might have avoided around 500 million tons of CO_2 emissions. In comparison, although the USA was fairly static with most of its coal-fired power plants seriously outdated, it has more efficient electricity dispatch. In China's ongoing twelfth Five-Year Plan (2011–2015), better dispatch patterns could be more important as opportunities for improvement through engineering approaches have been largely exhausted.

14/01847 Geostatistical modelling of a coal seam for resource risk assessment

Pardo-Igúzquiza, E. *et al. International Journal of Coal Geology*, 2013, 112, 134–140.

The evaluation of a coal seam for profitable extraction requires the estimation of its thickness and quality characteristics together with the spatial variability of these variables. In many cases the only data available for the estimation are from a limited number of exploration and feasibility drill holes. Spatial variability can be quantified by geostatistical modelling, which provides the basis for estimation (kriging). In cases where the spatial variability of the seam thickness and quality characteristics has a significant impact on how the coal is extracted and stored, geostatistical simulation may be preferable to geostatistical kriging methods. The aim of this paper is to present an improved approach to resource risk assessment by propagating the uncertainty in semi-variogram model parameters into the spatial variability of coal variables. The authors show that a more realistic assessment of risk is obtained when the uncertainty of semi-variogram model parameters is taken into account. The methodology is illustrated with a coal seam from north-western Spain.

14/01848 Technical and economic prospects of coal- and biomass-fired integrated gasification facilities equipped with CCS over time

Meerman, J. C. *et al. International Journal of Greenhouse Gas Control*, 2013, 16, 311–323.

This study analyses the impacts of technological improvements and increased operating experience on the techno-economic performance of integrated gasification (IG) facilities. The facilities investigated produce electricity (IGCC) or Fischer–Tropsch (FT) liquids with electricity as by-product (IG–FT). Results suggest that a state-of-the-art (SOTA) coal-fired IGCC without CO_2 capture has electricity production costs of 17 €/GJ (60 €/MWh) with the potential to decrease to 11 €/GJ (40 €/MWh) in the long term. Specific direct CO_2 emissions may drop from about 0.71 to 0.59 kg CO_2/kWh. If CO_2 is captured, production costs may increase to 23 €/GJ (83 €/MWh), with the potential to drop to 14 €/GJ (51 €/MWh) in the long term. As a result, CO_2 avoidance costs would decrease from 35 to 18 €/t CO_2. The efficiency penalty due to CO_2 capture and storage may decrease from 8.8%$_{pt}$ to 3.7%$_{pt}$. CO_2 emissions can also be reduced by using torrefied biomass (TOPS) instead of coal. Production costs of a SOTA TOPS-fired IGCC without CO_2 capture are 18–25 €/GJ (64–92 €/MWh). In the long term, this may drop to 12 €/GJ (44 €/MWh), resulting in CO_2 avoidance costs of 7 €/t CO_2. The greatest reduction in anthropogenic CO_2 emissions is obtained by using biomass combined with CCS. A SOTA TOPS-fired IGCC with CCS has, depending on the biomass price, production costs of 25–35 €/GJ (91–126 €/MWh) with CO_2 avoidance costs of 19–40 €/t CO_2. These values may decrease to 15 €/GJ (55 €/MWh) and 12 €/t CO_2 avoided in the long term. As carbon from biomass is captured, specific direct CO_2 emissions are negative and estimated at −0.93 kg CO_2/kWh for SOTA and −0.59 kg CO_2/kWh in the long term. Even though more carbon is sequested in the future concepts, specific emissions drop due to an increase in the energetic conversion efficiency of the future facilities. New technologies in IG-FT facilities have a slightly smaller impact on production costs. In the long term, production costs of FT liquids from coal may drop from 13 to 9 €/GJ if CO_2 is vented and from 15 to 10 €/GJ if CCS is applied. The use of TOPS results in 15–23 €/GJ (Vent) and 17–24 €/GJ (CCS) for SOTA facilities. These production costs may drop to 11–18 €/GJ (Vent) and 12–19 €/GJ (CCS) in the long term. Contrary to the IGCC cases, the coal-fired IG-FT facility shows the lowest CO_2 avoidance costs. The CO_2 emission of coal to FT liquids with CCS is, however, similar to gasoline/diesel production from crude oil.

Derived solid fuels

14/01849 Analysis of the errors associated with typical pulverized coal char combustion modeling assumptions for oxy-fuel combustion

Hecht, E. S. *et al. Combustion and Flame*, 2013, 160, (8), 1499–1509.

In computational fluid dynamic models of pulverized coal combustion, which often have complex, turbulent flows with millions of coal particles reacting, the char combustion sub-model needs to be computationally efficient. There are several common assumptions that are made in char combustion models that allow for a compact, computationally efficient model. In this work, often used single- and double-film simplified models are described, and the temperature and carbon combustion rates predicted from these models are compared against a more accurate continuous-film model. Both the single- and double-film models include a description of the heterogeneous reactions of carbon with O_2, CO_2 and H_2O, along with a Thiele-based description of reactant penetration. As compared to the continuous-film model, the double-film model predicts higher temperatures and carbon consumption rates, while the single-film model gives more accurate results. A single-film model is therefore preferred to a double-film model for a simplified, yet fairly accurate description of char combustion. For particles from 65 to 135 μm, in O_2 concentrations ranging from 12 to 60 vol.%, with either CO_2 or N_2 as a diluent, particle

temperatures from the single-film model are expected to be accurate within 270 K, and carbon consumption rate predictions should be within 16%, with greater accuracies for a CO_2 diluent and at lower bulk oxygen concentrations. A single-film model that accounts for reactant penetration and both oxidation and gasification reactions is suggested as a computationally efficient sub-model for coal char combustion that is reasonably accurate over a wide range of gas environments.

14/01850 Calcium-promoted catalytic activity of potassium carbonate for gasification of coal char: the synergistic effect unrelated to mineral matter in coal

Hu, J. *et al*. *Fuel*, 2013, 111, 628–635.

The purpose of this work is to investigate the synergistic catalysis between calcium species and K_2CO_3 for the char gasification. Graphite and four mineral-free chars including an anthracite coal char, a bituminous coal char, a lignite coal char and a pine wood char were gasified at 750 °C in a stream of steam/argon under atmospheric pressure. It was found that each of three calcium species ($Ca(OH)_2$, $Ca(CH_3COO)_2$ or $Ca(Ac)_2$, and $CaCO_3$) synergistically promoted the catalytic activity of K_2CO_3 for the gasification of all samples, and the extent of promotion was dependent on calcium species and carbon or char samples. The formation of a eutectic from the calcium species/K_2CO_3 catalyst was proved to be an important mechanism for its better catalytic effect. The presence of the organically bound calcium on the char was also likely to be responsible for the promoted catalytic gasification.

14/01851 Effect of reaction conditions on coke tumbling strength, carbon structure and mineralogy

Shen, F. *et al*. *Fuel*, 2013, 111, 223–228.

An experimental study was carried out to examine the effect of different reaction conditions on the changes in the tumbling strength of coke samples from two types of pilot-scale coke ovens. Cokes were reacted with different CO_2 concentration and different duration at the coke strength after reaction (CSR) test temperature of 1373 and 1573 K. Tumbling strength of the reacted cokes was measured using a typical CSR test routine. Carbon structure and mineralogy of cokes was measured using X-ray diffraction. Under the test conditions, temperature is shown to have the most significant impact on the modification of coke properties when compared to CO_2 concentration or the reaction duration. The tumbling strength of cokes reacted at 1573 K were found to be higher than the CSR value of the original cokes. With increasing temperature of the tests, low CSR cokes indicated a greater improvement of the tumbling strength. High tumbling strength cokes indicated high ordering of carbon structure and lesser amounts of reactive iron-bearing minerals. The effect of temperature on the improvement of tumbling strength can be related to the adverse effect of increased ordering of carbon structure and decreased proportion of iron-bearing phases on the coke reactivity, both being more notable in case of low CSR cokes. The study has implications on the efficient utilization of low premium coal resources and for the true assessment of coke performance in a blast furnace.

14/01852 Formation mechanism of carbon encapsulated Fe nanoparticles in the growth of single-/double-walled carbon nanotubes

Cui, C. *et al*. *Chemical Engineering Journal*, 2013, 223, 617–622.

The formation of carbon encapsulated Fe nanoparticles (Fe@C), in the process of growing single-walled/double-walled carbon nanotubes (S/DWCNTs) from methane was investigated by quantitatively analysing the samples at different reaction time. This study found that the ratio of Fe@C to the total Fe sustainably increased after the terminated growth of S/DWCNTs. The authors proposed that thin graphite layers produced in the middle stage of the reaction, as a mechanical barrier, covered the surface of MgO support and prevented Fe nanoparticles from contacting carbon source for the growth of S/DWCNTs via the root growth mode. These results suggested that the synthesis of desirable S/DWCNTs and undesirable Fe@C impurities was a consecutive process, not a parallelled one as proposed in many previous works. It provided useful information for the controlled synthesis of S/DWCNTs with high purity and high selectivity.

14/01853 Molecular oriented domains (MOD) and their effect on technological parameters within the structure of cokes produced from binary and ternary coal blends

Smędowski, Ł. and Krzesińska, M. *International Journal of Coal Geology*, 2013, 111, 90–97.

The aim of this work was to characterize molecular oriented domains in the cokes produced from binary and ternary blends of three bituminous Polish coals of varying carbon content: 82.7, 86.2 and 88.7 wt% and, consequently, of different caking propensities of the Roga index equal to 24, 63 and 77, respectively. The coals were collected from the Krupiński, Szczyglowice and Zofiówka mines, located in the Upper Silesian coal basin, Poland. They are commonly used in Polish coke-making industry. The samples were studied using transmission electron microscopy with the 002 dark field mode (002DF). As a result of these studies, an average area (S_{MOD}) of molecular-oriented domains (MOD) was determined for each sample. Values of the S_{MOD} parameter are discussed in relation to the composition of the blends. A distinct relationship between the Zofiówka coal content in a blend and the microtexture ordering degree of the cokes was found: the higher the Zofiówka coal content in a blend, the higher the S_{MOD} value. Values of S_{MOD} were related to the other structural parameters, i.e. to the average height of graphite-like crystallites, L_c, and to the percentage contribution of ordered structures, obtained using X-ray diffraction and Raman spectroscopy, respectively. The cokes containing 30–50% of the Zofiówka coal in a blend were found to have very well-ordered structures characterized by parameters close to those of the coke from the single Zofiówka coal reaching, dependently on a given factor, up to 80–99% of the values obtained for the coke from this strongly-caking coal. Values of S_{MOD} were also related to the technological indices of the cokes studied. Generally, the highly organized microtexture of the coal blend cokes was found to affect the *CRI* index: the lower is the value of S_{MOD} in the coke, the higher its *CRI*.

14/01854 Production of char from hornbeam sawdust and its performance evaluation in the dye removal

Ates, F. and Un, U. T. *Journal of Analytical and Applied Pyrolysis*, 2013, 103, 159–166.

Hornbeam sawdust was used as a biomass sample in the experiments involving char production. Within this purpose, a slow pyrolysis of the biomass sample was carried out in a fixed-bed reactor. The chemical characteristics of the chars obtained at 500, 600, 700 and 800 °C were identified by Fourier transform infrared spectroscopy, Brunauer–Emmett–Teller and scanning electron microscope analyses. The results of the analyses indicate that the properties of char greatly depend on the pyrolysis temperature. The higher the temperatures reached, the greater the amount of porous material obtained. In the second part of the study, four chars obtained through pyrolysis of hornbeam sawdust at different temperatures were used as an adsorbent for the removal of disperse orange 30 (DO30). Batch studies were performed to address various experimental parameters, such as pH, adsorbent dose, initial dye concentration, temperature and contact time for the removal of DO30. Dye was removed with the highest ratio decreasing both pH and the initial dye concentration. An increase in the amount of adsorbent, temperature and contact time also increased the dye removal efficiency. The greatest dye removal efficiency among the tested parameters was 71%. This was achieved using the 800 °C char at a concentration of 2.4 g L^{-1} and a solution pH of 2.

02 LIQUID FUELS

Sources, properties, recovery

14/01855 Comparison of paraffin nanoemulsions prepared by low-energy emulsification method for latent heat storage

Schalbart, P. and Kawaji, M. *International Journal of Thermal Sciences*, 2013, 67, 113–119.

In this study, oil-in-water nanoemulsions of refined and commercial grade paraffins have been prepared in the Tween60 + Span60/paraffin/water system by low-energy emulsification methods. A specific focus was on the increase of the energy density of these phase-change fluids for air conditioning applications. Concentrations up to 50 wt% have been obtained showing an equivalent specific heat capacity 3.5 times that of pure water. However, the degree of supercooling, though small in the bulk phase, has been found to be quite large in the emulsion.

14/01856 Direct mass spectrometry of tar sands: a new approach to bitumen identification

Flego, C. *et al*. *Fuel*, 2013, 111, 357–366.

The activities related to the evaluation of the organic fraction of tar sands are acquiring more importance from economical and technical points of view due to the increased variety of sample composition and origin. Conventionally, the analyses of bitumen in tar sands are based on preliminary extraction from the inorganic matrix and further characterization of physical and chemical features by means of different methods. A new approach to characterize the tar sand is now proposed, based on the direct insertion of tar sand into mass spectrometer chamber without any previous separation or treatment and further vaporization under vacuum at increasing temperature and

analysis of its components. Direct insertion probe–mass spectrometry (DIP–MS) allows separating the bitumen components from the solid inorganic matrix according to their boiling points up to masses of 700 m/z and directly analysing them in one only step, even if they are characterized by high boiling point, high steric hindrance or low solubility, that usually limit their evaluation by chromatographic methods. This new application of DIP–MS approach is here described on model materials and on a series of real tar sand samples coming from different geological areas. Differences are evidenced among the tar sands on the basis of the evolution of their mass spectra. The information so obtained was compared and confirmed with other analytical techniques that are commonly used for crude oil and bitumen characterization. This approach is proposed for an on-field application for fast screening of real samples in the perspective to acquire information on the most relevant organic species in the bitumen for comparative purposes and rough evaluation of the potentiality of tar sand fields.

14/01857 Evaluation and modeling of gas permeability changes in anthracite coals

Li, J. *et al. Fuel*, 2013, 111, 606–612.

The gas permeability of anthracite coal is altered as a result of the effective stress increase, the coal matrix shrinkage and the gas slippage that occur during the gas pressure depletion process. This paper describes an investigation of changes in the adsorbing-gas (CO_2) permeability of three anthracite coal cores (samples A, B and C). The changes in permeability under a constant confining stress condition (4.3 MPa) were found to be distinct for the three cores, and these observations are considered as the superimposed results of the three effects based on the following findings. During the gas pressure depletion: (a) the permeability is negatively proportional to the effective stress, and the slopes of the straight lines are near unity when the mean gas pressures are greater than 0.2–0.4 MPa; (b) the permeability increment induced by the gas slippage levels off to an approximately constant value (core A, 0.5 μD; core B, 0.6 μD; core C, 0.02 μD) when the mean gas pressure is greater than 0.8 MPa and subsequently becomes more significant at pressures less than 0.8 MPa; (c) the matrix shrinkage-induced permeability increment increases linearly for cores A and B but increases logarithmically for core C; and (d) the effect on the permeability of the effective stress predominates for core A, but for core C, the effect of the matrix shrinkage is most significant. Furthermore, an empirical model that predicts the adsorbing-gas permeability change was proposed as a function of the permeability increments caused by the effective stress, the matrix shrinkage and the gas slippage at each gas pressure under a constant confining stress condition, and can be mathematically expressed as: $k_{gt}=k_{oi}+\Delta k_{sli}(p_t)+\Delta k_{shr}(p_t)+\Delta k_{eff}(p_t)$. The results demonstrate that good agreement was achieved between the empirical models and the experimental data.

14/01858 Experimental study on the effects of sediment size and porosity on contaminant adsorption/desorption and interfacial diffusion characteristics

Fan, J.-y. *et al. Journal of Hydrodynamics, Ser. B*, 2013, 25, (1), 20–26.

The joint effects of the sediment size and porosity on the contaminant adsorption/desorption and interfacial diffusion characteristics were experimentally investigated. The adsorption of phosphorus (P) on the natural and artificial sediment suspensions was measured with respect to the P adsorption isotherms and kinetics in the experiment. The obtained adsorption isotherms for different grain-sized sediment suspensions fit well with the Langmuir equation, dependent on the initial aqueous concentration and sediment content. The P kinetic adsorption behaviours for cohesive fine-grained and non-cohesive coarse-grained sediment suspensions clearly show the size-dependent feature. On the other hand, the P kinetic release feature of a porous sediment layer is affected by not only the direct desorption of the uppermost sediments, but also the diffusivity in the pore-water within the underlying sediment layer, characterized by the sediment size and porosity, respectively. Furthermore, the temporal contaminant release from the permeable sediment layer into the overlying water column increases with the increasing flow velocity, while this enhancement in mediating the interfacial diffusion flux is somewhat insignificant in an immediate release stage, largely due to the resistance of the diffusive boundary layer on the hydrodynamic disturbance.

14/01859 Modification of heavy-oil rheology via alkaline solutions

Zhao, R. B. *et al. Journal of Petroleum Science and Engineering*, 2013, 103, 41–50.

Hamaca (Orinoco Belt, Venezuela) is considered here as a typical viscous and heavy oil whose rheology and recovery behaviour is potentially modified by diluents and aqueous solutions of alkali. Viscosity of dry Hamaca crude oil, mixtures of Hamaca and n-decane, as well as emulsified crude oil was measured *ex situ* and *in situ* (sand pack) as a function of temperature and shear rate. Hamaca crude oil exhibits temperature-dependent rheological behaviour. When between 30 and 50° C it is slightly shear thinning, whereas from 55 to 80° C, its properties are slightly shear-thickening. Shear stress sensitivity becomes greater as shear rate decreases. Crude oil rheological behaviour in a sand pack (single-phase flow) has similar trends as bulk crude-oil viscometer measurements. The viscosity of the crude oil decreases most significantly as the concentration of diluent (decane) increases from 0 to 6 wt% but the magnitude of viscosity reduction is less as diluent concentration increases from 10% to 33%. After mixing crude oil with aqueous alkaline silicate and carbonate solutions, viscosity decreases markedly due to formation of oil in water (o/w) emulsions. For sodium hydroxide, however, oil viscosity increases because of formation of water in oil emulsions. Given the encouraging changes in bulk oil properties, core flood recovery tests at different temperatures and flow rates were conducted. Alkaline flooding showed recovery of about 43% after 0.5 PV of injection and more than 60% with 5.6 PV of 1 wt% Na_2CO_3 solution. A significant fraction of the oil recovery occurred as o/w emulsion. The apparent relative permeability of the oil phase deviates markedly from the measurements for unemulsified oil.

14/01860 Oil shale formation in the Upper Cretaceous Nenjiang Formation of the Songliao Basin (NE China): implications from organic and inorganic geochemical analyses

Jia, J. *et al. International Journal of Coal Geology*, 2013, 113, 11–26.

Two oil shale layers are present in the Upper Cretaceous Nenjiang Formation of the Songliao Basin, representing excellent hydrocarbon source rocks. Their biomarker compositions provide evidence for a major contribution by aquatic organisms within the photic zone of the water column. Phytoplankton blooms were promoted by warm–humid climate, and lake eutrophication. Salinity stratification and anoxic bottom water conditions are indicated in the lower oil shale layer, whereas decreased salinity and partial oxygenation of the water column are evident in the upper oil shale layer. Moreover, an increase in sizes of alginite from the lower to the upper oil shale layer and enhanced telalginite concentrations is detected. Therefore, a stratified water column with high salinity and anoxic bottom water conditions contributes to organic matter (OM) preservation in the lower oil shale layer. In contrast, high bioproductivity in combination with OM preservation favoured by enhanced algae sizes and telalginite concentrations are suggested as the OM enrichment mechanisms in the upper oil shale layer. In addition, factors such as clay minerals, microbial activity, and detrital matter input cannot be ignored for their influence on OM enrichment. In this study, a preservation model within the lower oil shale layer and a productivity model within the upper oil shale layer are established. The models imply that excellent preservation is the major controlling factor for OM enrichment in the lower oil shale layer, whereas the high bioproductivity is the major controlling factor for OM enrichment in the upper oil shale layer. However, the combination of both factors for oil shale deposition must be considered.

Transport, refining, quality, storage

14/01861 A novel cascade fluidized-bed reactor assisted by hydrogen permselective membrane concept for improving gasoline productivity and selectivity in Fischer–Tropsch synthesis: a simulation study

Bayat, M. and Rahimpour, M. R. *Journal of Natural Gas Science and Engineering*, 2013, 13, 20–29.

In this work, a novel cascade fluidized-bed reactor assisted via Pd/Ag membrane layer for Fischer–Tropsch synthesis is simulated, mathematically. In the first catalyst bed, the synthesis gas is partially converted to hydrocarbons in water-cooled reactor which is a fluidized bed. In the second bed which is a membrane assisted fluidized-bed reactor, the reaction heat is used to preheat the feed gas to the first bed. Due to the decrease of H_2/CO to values far from the optimum reactant ratio, the membrane concept is suggested to control the hydrogen addition. This reactor configuration solves some observed weakness of conventional reactor such as high pressure drop, heat transfer problem and internal mass transfer limitations. Because of the inherent complexity of dense gas-particles flows, the two-phase theory in bubbling regime of fluidization is used to model and simulate the proposed reactor. The simulation results show an enhancement of gasoline yield, a main decrease in undesirable products formation and a favourable temperature profile along the proposed concept.

14/01862 Experimental study on the stability of the foamy oil in developing heavy oil reservoirs

Liu, P. *et al. Fuel*, 2013, 111, 12–19.

In the process of natural energy depletion, foamy oil is characterized of high oil viscosity, low production gas-to-oil ratio, high daily production rate; relatively slow production decline rate and high primary recovery factor (compared with conventional heavy oil). The stability of the foam becomes the dominant factor that determines the life of the 'foamy oil'. To quantify the main factors affecting the stability of the foam, a high-temperature–high-pressure visualized experiment model for foamy oil stability test was developed. A series of experiments was conducted to evaluate the performance of the foam stability under different conditions, including temperature, dissolved gas oil ratio, pressure decline rate and the pore sizes. As indicated by the test results, the stable foamy oil exists only if the reservoir temperature is lower than 70 °C. The initial dissolved gas oil ratio was higher than 4.23 m^3/m^3 and the pressure depletion rate was higher than 0.0018 MPa/min. It was also concluded that as the pore sizes of the porous media becomes closer to the actual reservoir pore size, the foam can last longer, which indicates that the 'foamy oil' will exist for a long time during the reservoir development. The experimental results above have been used to guide the development of Block MPE-3 in Venezuela.

14/01863 Geomechanics of thermal viscous oil production in sandstones

Shafiei, A. and Dusseault, M. B. *Journal of Petroleum Science and Engineering*, 2013, 103, 121–139.

Over 7 Tb of viscous oil (heavy oil, extra heavy oil, and bitumen) are trapped in sandstones or unconsolidated sand formations around the world, mainly in Canada, Venezuela and Russia. To date, only cold flow methods and steam injection processes have achieved commercial success in accessing this immense resource. This paper highlights the definitions, geology and origins, and geographical distribution of the viscous oil resources in the world, and then describes the approaches and physical mechanisms of the major commercialized viscous oil production methods being practiced around the world. Approaches to calculating thermally induced stresses are presented, as well as discussions of thermomechanical issues associated with commercial thermal processes. Then, thermal, physical, and geomechanical properties of sandstone under high temperature and pressure are investigated, based on field and laboratory data. An important factor is the change in rock properties that takes place because of the large thermally-induced stresses. Finally, a practical example of thermal geomechanics effects during thermal oil production operations (the example of steam-assisted gravity drainage) is demonstrated, emphasizing that thermal oil production methods change reservoir rock behaviour. Under elevated temperature and pressure, large changes in porosity, permeability and compressibility occur; hence, the reservoir response evolves in time, a factor generally ignored in simulation. Whereas these geomechanical changes are largely beneficial as they tend to accelerate recovery rates, some difficult operational issues may arise, including casing shear, breach of reservoir seal, and excessive heat loss.

14/01864 High viscosity effects on characteristics of oil and gas two-phase flow in horizontal pipes

Zhao, Y. *et al. Chemical Engineering Science*, 2013, 95, 343–352.

The flow characteristics of high viscosity oil and gas flow show several significant differences with those of low viscosity liquid. Effects of high viscosity oil on characteristics of oil and gas flow are identified. The present experiments are performed on the flow facility which consists of a test section of 26 mm inside diameter and a 5.5 m long horizontal pipe. A range of liquid viscosity from 1000 to 7500 cP is investigated. The superficial oil and gas velocities vary from 0.06 to 0.5 m/s and from 0.3 to 12.0 m/s, respectively. The resulting flow patterns are identified by electrical capacitance tomography (ECT) and confirmed by videos recorded during the experiments. The pressure and liquid holdup data are obtained by using pressure transducers and ECT system. The experimental results are compared with existing models and show significant discrepancies between low and high viscosity liquid and gas flows.

14/01865 Modeling and validation of pressure propagation in drilling fluids pumped into a closed well

de Oliveira, G. M. *et al. Journal of Petroleum Science and Engineering*, 2013, 103, 61–71.

This study presents a mathematical model to simulate the pressure propagation that takes place when a drilling fluid is pressurized within a closed pipe-annular geometry. The model assumes that fluid motion is one-dimensional and weakly compressible and the system is considered isothermal. The model comprises the continuity and momentum balance equations, which are iteratively solved by the method of characteristics. The proposed model can be applied to both Newtonian and Bingham fluids. The viscous effect is considered in the model using the friction factor approach. Pressure values obtained from the model are compared to experimental data from an earlier study for a Newtonian (water) and two drilling fluids. Not only the magnitudes but also the oscillation frequencies of the measured and computed values show a qualitatively fair agreement for both kinds of fluid. Both measured and computed values show that pressure is not fully transmitted in drilling fluids. Three dimensionless numbers are identified as the model governing parameters. A model sensitivity analysis shows that pressure propagation can be enhanced by combining the governing parameters.

14/01866 Numerical simulation of thermal and reaction fronts for oil shale upgrading

Youtsos, M. S. K. *et al. Chemical Engineering Science*, 2013, 94, 200–213.

This paper analyses reaction and thermal front development in porous reservoirs with reacting flows, such as those encountered in oil shale upgrading. A set of dimensionless groups and a one-dimensional code are developed in order to investigate the important physical and chemical variables of such reservoirs when heated by *in situ* methods. Theory necessary for this study is presented, namely shale decomposition chemical mechanisms, governing equations for multiphase flow in porous media and necessary closure models. Plotting the ratio of the thermal front speed to the fluid speed allows one to infer that the reaction front ends where this ratio is at a minimum. The reaction front follows the thermal front closely, thus allowing assumptions to be made about the extent of decomposition solely by looking at thermal front progression. Furthermore, this sensitivity analysis showed that a certain minimum permeability is required in order to ensure the formation of a travelling thermal front. Compared to varying deposit porosities and kerogen activations energies, varying temperature, pressure and permeability are more important.

14/01867 On the influence of filling level in CFRP aircraft fuel tank subjected to high velocity impacts

Artero-Guerrero, J. A. *et al. Composite Structures*, 2013, 107, 570–577.

In this work, the process of impact that takes place in a partially filled carbon fibre-reinforced plastic (CFRP) aircraft fuel tank is analysed, performing a numerical simulation, in order to understand the response of the composite laminated structure. The commercial finite-element code LS-DYNA v.R7 has been used to simulate a hydrodynamic ram event created by a steel spherical projectile impacting a partially water-filled woven CFRP square tube using two different approaches (MM-ALE and SPH). The intralaminar and interlaminar damage have been taken into account implementing a user subroutine and by means of a cohesive interaction, respectively. Once the numerical model is validated using available experimental data, the effect of the filling level in the failure of the tank is analysed in detail taking advantage of the information provided by the numerical model.

14/01868 Operational optimization of crude oil distillation systems using artificial neural networks

Ochoa-Estopier, L. M. *et al. Computers & Chemical Engineering*, 2013, 59, 178–185.

A new methodology for optimizing heat-integrated crude oil distillation systems is proposed in this work. The new procedure considers an artificial neural networks model for representing the distillation column. Models of the distillation column and the associated existing heat exchanger network are incorporated in an optimization framework to systematically determine the operating conditions that improve the overall process economics. Of particular interest is the problem of optimizing the net value of the products obtained from the column by increasing the yield of higher-value products at the expense of less valuable products, while taking into account feasibility of the distillation specifications, heat recovery, energy and equipment constraints. A two-stage procedure is applied to first optimize the column operating conditions based on minimum utility requirements. In the second stage the heat exchanger network is designed.

14/01869 Optimization of oil production under gas coning conditions

Hasan, A. *et al. Journal of Petroleum Science and Engineering*, 2013, 105, 26–33.

Typically, a well is produced with a constant oil rate with constant gas–oil ratio during the subcritical phase, i.e. before gas breakthrough. The presence of gas coning in production wells may reduce the oil production. The decline in the oil rate will be followed by an increase in the well head pressure. From an economical and operational point of view, this condition may be undesirable for several reasons: the gas price is much lower than the oil price, the afflicted well may be abandoned early, and the gas handling capacity often is a constraint. Therefore, there is an incentive to produce such wells in their subcritical phase for an extended period of time. In this paper, the gas coning process in a gas–oil reservoir completed with a single horizontal well is analytically modelled, simulated, and analysed applying a non-linear control approach. The horizontal well model which describes the interaction between the well and the reservoir may

be cast into a boundary control problem of the porous media equation with two boundary conditions: a homogeneous Neumann's boundary condition describing no-flow at the outer boundary of the reservoir, and a non-linear boundary condition describing the well production rate. A well rate controller for the boundary control problem is designed using the backstepping method. The controller holds some formal performance guarantees and requires information on the gas–oil contact at the well heel only. Furthermore, the controller has a tuning parameter which can be used to maximize a suitable performance measure, e.g. the net present value. The controller is evaluated using a detailed Eclipse simulator of a gas coning reservoir. Simulation results show significant improvement of production profit of the proposed method compared to a conventional method which usually uses a constant rate until gas breakthrough.

14/01870 Pipe dope as a source of oil and gas formation damage

De Franceschi, E. *et al. Journal of Natural Gas Science and Engineering*, 2013, 12, 65–73.

From the beginning of the oil and gas industry, thread-compound products (commonly known as 'pipe dope' in the vernacular) have been used to join the threaded connections of tubing and casing tubes. These compounds can carry from 19% to 25% of heavy inorganic particles (such as lead, zinc, lithium and graphite among others) which provide the sealing properties to the pipe connections throughout a wide range of temperatures. Dopes are hydrocarbon resistant for the obvious reasons and provide lubrication to the connections during the thread engagement, avoiding galling while maintaining the connection's mechanical integrity. However, the doping practice involves the manual application of the lubricant in a fashion that is rudimentary, non-systematic and unquantifiable. Any excess quantity of dope exuded during the make-up of connections could result in a series of problems inside the well, such as the clogging of sandscreens, valves and heads of the perforating guns. The excess of dope accumulated inside the tubing can also cause wire-line failures, reading problems of the logging tools during the data acquisition and completion fluids contamination. But the most severe and almost irreversible problem that the thread compound could bring inside the well is the damage caused to the near-well zone, because it would be difficult to remove this with either water- or hydrocarbon-based solvents. This paper looks at the manner with which pipe dope is applied. Laboratory, field and core testing has been employed to quantify the effects of the material. It is concluded that pipe dope can cause severe damage in producing wells and, almost certainly, severe damage in injection wells.

14/01871 Practical process design for in situ gasification of bitumen

Kapadia, P. R. *et al. Applied Energy*, 2013, 107, 281–296.

The province of Alberta, Canada hosts an estimated 170 billion barrels of crude bitumen reserves in the Athabasca, Cold Lake and Peace River deposits. These reserves are commercially recovered through surface mining or *in situ* recovery methods. Most of the produced bitumen is converted in surface upgraders to synthetic crude oil (SCO), a 31–33°API oil product. Next, SCO is converted to transportation fuels, lubricants and petrochemicals in conventional refineries and petrochemical industries. *In situ* recovery or mining as well as bitumen upgrading and refining are energy intensive processes that generate huge volumes of acid gas, consume massive volumes of water, and are costly. Bitumen upgrading requires hydrogen, and currently most of it is produced by steam reforming of methane. Alternatively, hydrogen can be generated by *in situ* gasification of bitumen. *In situ* gasification of oil sands is potentially more energy efficient with reduced emission to atmosphere since acid gases are sequestered to some extent in the reservoir. Also, water usage is lowered and heavy metals and sulfur compounds in the bitumen tend to remain downhole since the main product is gas. The objective of this research was to understand and optimize hydrogen generation by *in situ* gasification from bitumen reservoirs. The central idea was to recover energy from the reservoir in the form of hydrogen and bitumen. *In situ* combustion has been attempted in the field, in a pilot run at Marguerite Lake. In this pilot, the produced gas contained up to 20 mol% of hydrogen. In this study, the Marguerite Lake Phase A main-pattern *in situ* combustion pilot was history-matched as a basis to understand a field-operated recovery process where *in situ* gasification reactions occur. Based on Marguerite Lake *in situ* combustion pilot observations, a new *in situ* bitumen gasification process, based on a steam-assisted gravity drainage (SAGD) well configuration, was designed and compared with conventional SAGD on the basis of energy investment, emission to atmosphere and water usage. The results show that the amount of energy produced per unit of energy invested for the *in situ* gasification process was greater than the steam alone recovery process with less than half the water usage. The cyclic injection of steam and oxygen as compared to steam injection alone can permit design of oil-alone to oil and syngas production processes.

14/01872 Reservoir modeling of shale formations

Mohaghegh, S. D. *Journal of Natural Gas Science and Engineering*, 2013, 12, 22–33.

Economic production from shale has been intimately tied to hydraulic fracturing since the first signs of success in Barnet Shale in the late 1990s. The introduction of horizontal wells and multi-stage hydraulic fracturing was met by a huge move by operators toward developing shale formations that were mainly ignored in the past. Today, using pad drilling, multiple horizontal wells share surface facilities and infrastructure, a development that minimizes the industry's environmental footprint. To understand production from shale reservoirs one must understand the network of natural fractures in the shale and the role of hydraulically induced fractures and their interaction. Hydraulic fracturing has been around and been studied by engineers for decades. Analytical, numerical and data-driven models have been built to explain their behaviour and contribution to flow. Contribution of natural fracture networks to storage and flow in carbonate (and some sandstone) reservoirs had led to the development of techniques to study and model them. Since they are the predominant source of porosity and permeability in shale, more attention has been focused on their characteristics in the recent years. Studies of methane production from coal seams in the mid-1980s provided insights on sorption as a storage mechanism and desorption and diffusion as a transport phenomenon in reservoirs that came to be known as coalbed methane. Today, production from shale is mainly modelled based on lessons learned in the past several decades where all the above techniques are integrated to create the modern shale reservoir models. The coupling of hydraulic fractures and natural fracture networks and their integration and interaction with the shale matrix remains the major challenge in reservoir simulation and modelling of shale formations. This article reviews the methods used by scientists and engineers in recent years to understand the complexities associated with production from shale. This will shed light on the commonly held belief that there is much to be learned about this complex resource and that the best days in understanding and modelling how oil and gas are produced from shale are still ahead of us.

14/01873 Supplying synthetic crude oil from Canadian oil sands: a comparative study of the costs and CO_2 emissions of mining and in-situ recovery

Méjean, A. and Hope, C. *Energy Policy*, 2013, 60, 27–40.

High crude oil prices and the eventual decline of conventional oil production raise the issue of alternative fuels such as non-conventional oil. This paper describes a simple probabilistic model of the costs of synthetic crude oil produced from Canadian oil sands. Synthetic crude oil is obtained by upgrading bitumen that is first produced through mining or *in situ* recovery techniques. This forward-looking analysis quantifies the effects of learning and production constraints on the costs of supplying synthetic crude oil. The sensitivity analysis shows that before 2035, the most influential parameters are the learning parameter in the case of *in situ* bitumen and the depletion parameter in the case of mined bitumen. After 2035, depletion dominates in both cases. The results show that the social cost of CO_2 has a large impact on the total costs of synthetic crude oil, in particular in the case of synthetic crude oil from *in situ* bitumen, due to the carbon intensity of the recovery techniques: taking into account the social cost of CO_2 adds more than half to the cost of producing synthetic crude oil from mined bitumen in 2050 (mean value), while the cost of producing synthetic crude oil from *in situ* bitumen more than doubles.

Economics, business, marketing, policy

14/01874 A systematic laboratory study on an anticorrosive cool coating of oil storage tanks for evaporation loss control and energy conservation

Zhang, W. *et al. Energy*, 2013, 58, 617–627.

The composition and manufacturing process of a three-layer anti-corrosive cool coating for oil storage tanks are introduced. The optical, indoor thermal and physicochemical properties were systematically investigated. In addition, the outdoor cooling effect and the reduction of evaporation losses of crude oil were predicted. The coating developed has high solar reflectance and thermal emittance and thus good indoor and outdoor temperature reduction effects. The unique structural design and the careful selection of ingredients endow the coating with low thermal conductivity and good resistance to dirt, weather, salt spray and chemicals. The selected epoxy functional saline couple agent creates a chemical bridge between the coating's binder and the surface of carbon steel substrates and improves the adhesion of the coating.

14/01875 An application of a multi-agent auction-based protocol to the tactical planning of oil product transport in the Brazilian multimodal network

Banaszewski, R. F. *et al. Computers & Chemical Engineering*, 2013, 59, 17–32.

The transportation planning of oil products in Brazil's multimodal network is a complex problem that involves various negotiations between decentralized entities in order to agree on which products to transfer, their amounts, and the allocation of shared resources. Due to such complexity, there is a clear need for a decision support tool. This paper presents a model for solving this problem based on a new multi-agent auction protocol. The developed model is used to solve a real scenario of the Brazilian oil supply chain in a multi-level topological approach.

14/01876 Development of new type curves for production analysis in naturally fractured shale gas/tight gas reservoirs

Xu, B. *et al. Journal of Petroleum Science and Engineering*, 2013, 105, 107–115.

As a result of ultra-low rock permeability and hydraulic fracturing, both shale gas and tight gas production exhibit long-term transient and linear flow behaviour. Previous studies have introduced the type curves for linear flow reservoir and assumed that the production is dominated by the stimulated reservoir volume (SRV). Later, the type curves were extended to include the production contribution from the unstimulated region, which has been assumed to be a homogeneous system. At present, no type curves have been developed for naturally fractured shale gas/tight gas reservoirs in which the unstimulated region has double porosity flow behaviour. In this study, the authors have developed new analytical solutions for shale gas/tight gas reservoirs with multi-stage fractured horizontal well in order to account for the unstimulated region as a dual porosity system. The solutions are more general for type curve analysis and applicable in both homogeneous and naturally fractured reservoirs. Numerical models were used to validate the analytical solutions and obtained an excellent agreement. The authors have also developed new type curves for shale gas/tight gas evaluation. The flow regimes are identified to show linear flow and transition flow alternately, and are more complicated than the assumption of homogeneous unstimulated reservoir in late period. The authors have compared the new type curves with the curves based on SRV and Brohi's solutions. It is concluded that the double porosity behaviour of unstimulated region has a positive effect on production even if the fracture permeability is in the order of matrix permeability and the matrix bulk shape factor is low.

14/01877 Do oil prices predict economic growth? New global evidence

Narayan, P. K. *et al. Energy Economics*, 2014, 41, 137–146.

This study tested whether oil price predicts economic growth for 28 developed and 17 developing countries. Predictability tests were used that account for the key features of the data, namely, persistency, endogeneity, and heteroskedasticity. This analysis considers a large number of countries, shows evidence of more out-of-sample predictability with nominal than real oil prices, finds in-sample predictability to be independent of the use of nominal and real prices, and reveals greater evidence of predictability for developed countries.

14/01878 Modeling and performance prediction for water production in CBM wells of an eastern India coalfield

Agarwal, A. *et al. Journal of Petroleum Science and Engineering*, 2013, 103, 115–120.

Dewatering of coalbed methane (CBM) reservoirs is a very important part of methane production. Efficient production depends very much on the proper designing of the wells. In this study, a comprehensive testing was conducted on 17 wells of a particular block in eastern India and a general reservoir flow equation modelled. Prediction of the water flow potential of a particular well using the derived flow equation helps in monitoring the variables of the artificial lift facility. The outcome of work can be used comprehensively to predict the future water and gas flow rates of simulated wells under the designed test.

14/01879 Oil demand shocks reconsidered: a cointegrated vector autoregression

Kolodzeij, M. and Kaufmann, R. K. *Energy Economics*, 2014, 41, 33–40.

This study reconsiders the conclusions about the importance of oil demand shocks and the unimportance of supply shocks reported in an earlier study by Kilian. The authors investigate whether the proxy for worldwide real economic activity, dry bulk maritime freight costs, represents anything more than transportation costs by analysing the relation between these costs and oil prices. The meaning of this variable is critical because transportation costs appear on both sides of the equations estimated by Kilian, directly as dry bulk maritime freight costs and as part of the measure for oil prices. The authors also investigate the effects of representing oil supply with an aggregate of OPEC and non-OPEC production because they likely use different criteria to choose output. Finally there is an investigation into Kilian's use of the first difference of supply while the other variables in his model are represented as levels. The results suggest that OPEC and non-OPEC nations use different criteria to set output and that reductions (increases) in OPEC production raise (lower) oil prices. The elements of the cointegrating relations, their loadings, and impulse response functions suggest that the positive relation between dry bulk maritime freight costs and oil prices simply represents the effect of higher oil prices on transportation costs. Sensitivity analyses suggest that these differences are caused by including transportation costs in the measure of oil prices, aggregating OPEC and non-OPEC productions, and using a very long lag length to estimate the vector autoregressive. Together, these results suggest that conclusions about the importance of demand shocks and the unimportance of supply shocks are not robust to alternative specifications that are consistent with many empirical findings about the world oil market.

14/01880 Oil price risk exposure: the case of the U.S. travel and leisure industry

Mohanty, S. *et al. Energy Economics*, 2014, 41, 117–124.

This study investigate the oil price risk exposure of the US travel and leisure industry by using the Fama–French–Carhart's four-factor asset pricing model augmented with the oil price risk factor. The results of this study suggest that oil price sensitivities vary significantly across six subsectors: airlines, gambling, hotels, recreational services, restaurants and bars, and travel and tourism. The extent of the exposure is generally negative, but it is particularly significant for a number of subsectors including airlines, recreational services and restaurants and bars. Oil price risk exposures also vary considerably over time. In particular, the 2007–2009 recession triggered by the US subprime lending crisis has significantly contributed to the oil price risk exposure of airline industry. These results should be of interest to financial analysts, corporate executives, money managers, regulators, and policy makers.

14/01881 Procurement planning in oil refining industries considering blending operations

Oddsdottir, T. A. *et al. Computers & Chemical Engineering*, 2013, 58, 1–13.

This paper addresses procurement planning in oil refining, which has until now only had limited attention in the literature. The authors introduce a mixed integer non-linear programming model and develop a novel two-stage solution approach, which aims at computational efficiency while addressing the problems due to discrepancies between a non-linear and a linearized formulation. The proposed model covers realistic settings by allowing the blending of crude oil in storage tanks, by modelling storage tanks and relevant processing units individually, and by handling more crude oil types and quality parameters than in previous literature. The developed approach is tested using historical data from Statoil A/S as well as through a comprehensive numerical analysis. The approach generates a feasible procurement plan within acceptable computation time, is able to quickly adjust an existing plan to take advantage of individual procurement opportunities, and can be used within a rolling time horizon scheme.

14/01882 The elasticity of demand for gasoline in China

Lin, C.-Y. C. and Zeng, J. *Energy Policy*, 2013, 59, 189–197.

This paper estimates the price and income elasticities of demand for gasoline in China. The estimates of the intermediate-run price elasticity of gasoline demand range between −0.497 and −0.196, and the estimates of the intermediate-run income elasticity of gasoline demand range between 1.01 and 1.05. The authors also extend previous studies to estimate the vehicle miles travelled elasticity and obtain a range from −0.882 to −0.579.

14/01883 What is energy efficiency and emission reduction potential in the Iranian petrochemical industry?

Mohammadi, A. *et al. International Journal of Greenhouse Gas Control*, 2013, 12, 460–471.

In this study, the prospects of energy efficiency potential, clean development mechanism (CDM) and carbon income up to and beyond 2012 are investigated in the petrochemical industries of Iran as a major oil-producing country. This paper addresses four questions: (1) the greenhouse gas (GHG) emissions in Iranian petrochemical complexes, (2) the most energy-consuming processes, (3) units with the highest energy efficiency potentials and (4) potentials of CDM or similar carbon projects based on post-2012 scenarios. The petrochemical processes are investigated in two categories of non-polymeric and polymeric productions. Based on capital expenditure, economic saving, simple payback period, CO_2 equivalent emissions, and the level of technology transfer, the attractiveness of energy efficiency measures is assessed and CDM potentials are investigated. Meanwhile, the impact of the recently deregulation of national energy-prices is examined. The results reveal that the three main non-polymeric (ammonia, urea and methanol) processes in Iran offer the most opportunity for energy

efficiency improvement and carbon-market potentials followed by the polymeric processes in units with outdated technology. The studied petrochemical units indicate over 2.53 million tons CO_2-eq/year potential reduction in GHG emissions and natural gas conservation of 1100 million-m^3/year. Nonetheless, more detailed energy-auditing for the entire Iranian petrochemicals is required for a comprehensive analysis.

14/01884 Will Venezuelan extra-heavy oil be a significant source of petroleum in the next decades?

de Sena, M. F. M. *et al. Energy Policy*, 2013, 61, 51–59.

Unconventional oil resources are needed to complement petroleum supply in the next decades. However, given the restrictions that pertain to the production of these resources, this article evaluates the availability of Venezuelan unconventional oil for helping meet the future worldwide petroleum demand. Venezuela has the world's second-largest oil reserves, but the majority of it is unconventional extra-heavy oil from the Orinoco oil belt. The perspective of Venezuelan production, the ways in which the state oil company will raise funds for planned investments and the future oil price predictions are used to assess Venezuela's ability to serve as a source of unconventional oil in the coming years. Findings indicate that Venezuelan crude oil will be increasingly able to provide part of the marginal petroleum supply at a level predicted in global scenarios but short of that predicted by the country's government. Operational difficulties and the effort to raise financial resources for the oil production in the oil belt require urgency in overcoming difficulties. As conventional production in Venezuela will stabilize in the coming years and the country is dependent on oil production, Venezuela will rely on extra-heavy oil extraction to ensure increased oil production and the stabilization of internal accounts.

Derived liquid fuels

14/01885 CO_2 implications of coal-to-liquids (CTL) plants

Mantripragada, H. C. and Rubin, E. S. *International Journal of Greenhouse Gas Control*, 2013, 16, 50–60.

In this study, plant-level techno-economic models are developed and applied to systematically evaluate the performance, emissions and costs of a much broader range of coal-to-liquids (CTL) plant designs than have previously been studied. These include two plant configurations (a liquids-only plant similar to current commercial technology, and a co-production plant producing both liquids and electricity), two types of coal gasification systems (slurry-feed and dry-feed gasifiers), and three types of coal feedstock (bituminous, sub-bituminous and lignite). For all 12 designs, the additional cost of carbon dioxide capture and storage (CCS) and the effects of a price or tax on plant-level CO_2 emissions, as well as the option of sale of CO_2 for enhanced oil recovery (EOR), also are studied. The potential of the co-production configuration to reduce overall CO_2 emissions by displacing conventional pulverized coal power plants is also investigated. The economic feasibility of CCS depends strongly on the CO_2 price/tax and electricity selling price. In general for liquids-only plants, CCS is the more economical option than paying even the 'low' CO_2 tax of $20/tonne for the non-CCS cases. For co-production plants, a higher CO_2 tax is required to make CCS feasible because of the foregone revenues from electricity sales (due to CCS energy requirements). EOR options generally have the lowest cost of liquids produced, in the range of $45–$100/barrel, across all cases. Co-production is more efficient than the separate production of liquids and power, and this difference in efficiency increases with the addition of CCS. This advantage can be utilized to achieve a net reduction in overall CO_2 emissions.

14/01886 Design and control of a reactive-distillation process for esterification of an alcohol mixture containing ethanol and *n*-butanol

Wu, Y.-C. *et al. Computers & Chemical Engineering*, 2013, 57, 63–77.

This paper presents an economical design flowsheet and overall control strategy for simultaneous esterifications of ethanol and *n*-butanol mixtures with acetic acid. In this work, a difficult-to-design reactive-distillation (RD) process, classified as mixed Type-II/Type-III system, has been studied. After comparing three alternative design flowsheets, an indirect-sequence design containing a RD column, a top decanter, and a stripper gives significantly lower total annual cost and energy consumption than the other two designs. In the control strategy development, conventional inventory control with RD bottom level controlled by manipulating RD bottom flow shows that this process would exhibit multiple steady-states. An improved inventory control strategy with a rather unusual pairing by controlling this level using reboiler duty is proposed to alleviate this complex dynamic behaviour. The dynamic results show that the proposed plant-wide control strategy is capable of holding product specifications despite disturbances from throughput and feed composition changes.

14/01887 GTL (gas to liquid) and RME (rapeseed methyl wster) combustion analysis in a transparent CI (compression ignition) engine by means of IR (infrared) digital imaging

Mancaruso, E. *et al. Energy*, 2013, 58, 185–191.

In the present paper, infrared measurements were performed in order to study the behaviour of biofuels combustion in a transparent Euro 5 diesel engine operating in premixed mode. Commercial diesel fuel, gas-to-liquid (GTL) and rapeseed methyl ester (RME) biofuels have been used. An elongated single-cylinder transparent engine equipped with the multi-cylinder head of commercial passenger car and common rail injection system was used. A sapphire window was set in the bottom of the combustion chamber, and a sapphire ring was placed in the upper part of the cylinder. Measurements were carried out through both accesses by means of high-speed infrared digital imaging system. An infrared camera was able to detect the emitted light in the wavelength range of 1.5–5 μm. Infrared imaging permitted the acquisition of a larger amount of information than ultraviolet and visible light cameras. In particular, the infrared camera was used for the characterization of injection and combustion process. By analysing the infrared images it was possible to identify the seven jets of vaporized fuel that react with air in the bowl. During the late combustion phase, the image showed a good capability to follow the hot burned gas both in the bowl and above the piston. The infrared camera has shown high sensibility, permitting one to follow carefully the soot oxidation process within the cylinder. The GTL shows an advance of about an 8° crank angle in the evolution of combustion process with respect to the RME. On the contrary, a longer chemical activity has been detected for the latter biofuel. Finally, the infrared camera has been shown to be a very useful tool to characterize the combustion process for over a long time period, allowing high quality results. Clear images of the reactions that happen in the combustion chamber and above the piston head were acquired even if the optical windows were obscured by the soot produced from the previous combustion cycles.

14/01888 Pilot plant validation of a rate-based extractive distillation model for water–ethanol separation with the ionic liquid [emim][DCA] as solvent

Quijada-Maldonado, E. *et al. Chemical Engineering Journal*, 2013, 223, 287–297.

The separation of water–ethanol mixtures is an important research topic due to the use of ethanol as a replacement of fossil fuels. Extractive distillation with ionic liquids has been proposed as a promising and attractive technology to separate this mixture. However, ionic liquids show high viscositites and this could markedly decrease the mass transfer efficiency of the column. A rate based-model is able to predict and evaluate mass transfer efficiencies while only knowing the physical and transport properties of the system in question. With the objective of validating a developed rate-based model for the separation of water–ethanol mixtures by using 1-ethyl-3-methylimidazolium dicyanamide and ethylene glycol as solvents and investigating the effect of the solvent physical properties on mass transfer efficiency, an extractive distillation pilot-plant equipped with Mellapak® 750Y was constructed and operated in continuous mode. It was found that the rate-based model predicts the performance of this pilot plan very well for all the studied conditions within a 10% relative error. Slightly more optimistic water contents of the distillate stream were predicted and experimentally the ionic liquid produced lower water contents than ethylene glycol. The use of this ionic liquid provides higher mass transfer efficiencies for all the studied solvent-to-feed ratios. Finally, increasing the solvent-to-feed ratio enhances the mass transfer efficiencies for both solvents and effects of liquid viscosity decreasing the mass transfer efficiency are observed in the rectifying section of the extractive distillation column.

14/01889 Transesterification of palm oil with methanol in a reactive distillation column

Prasertsit, K. *et al. Chemical Engineering and Processing: Process Intensification*, 2013, 70, 21–26.

The higher feedstock and processing costs for biodiesel production can be reduced by applying reactive distillation (RD) in transesterification process. The effects of reboiler temperature, amount of KOH catalyst, methanol to oil molar ratio and residence time on the methyl ester purity were determined by using a simple laboratory-scale RD packed column. The results indicated that from the empty column, the system reached the steady state in 8 h. Too high reboiler temperature and the amount of catalyst introduce more soap from saponification in the process. The optimal operating condition is at a reboiler temperature 90 °C, a methanol-to-oil molar ratio of 4.5 : 1.0, KOH of 1 wt% with respect to oil and 5 min of residence time in the column. This condition

requires the fresh feed methanol 25% lower than in the conventional process and produces 92.27% methyl ester purity. Therefore this RD column can be applied in small or medium biodiesel enterprise.

14/01890 Two step copper impregnated zinc oxide microball synthesis for the reduction of activation energy of methanol steam reformation

Danwittayakul, S. and Dutta, J. *Chemical Engineering Journal*, 2013, 223, 304–308.

Cu/ZnO microball catalysts were prepared by a two-step process, where ZnO nanorods supports were first grown hydrothermally followed by the impregnation of copper nanoparticles. Catalytic activities for methanol steam reforming by using Cu/ZnO microball were found to increase with higher copper content. Addition of urea during the metal impregnation process was found to enhance the methanol steam reforming catalytic activity attributed to the larger surface area of the catalyst. Activation energies of synthesized catalyst and CuZnAl commercial catalyst were calculated from the Arrhenius plots of the rate of reaction and were found to affect hydrogen yield. The lowest activation energy of 4.74 kJ mol^{-1} was achieved for the optimized catalyst which was half of the activation energy of commercial catalysts.

03 GASEOUS FUELS

Sources, properties, recovery, treatment

14/01891 A hydrous pyrolysis study to ascertain how gas yields and the extent of maturation for a partially matured source rock and bitumen in isolation compared to their whole source rock

Uguna, C. N. *et al. Journal of Analytical and Applied Pyrolysis*, 2013, 103, 268–277.

In order to ascertain whether kerogen and the heavy oil or bitumen generated during the initial stages of source rock maturation then go on to produce similar gas yields compared to the natural situation when they are present in source rocks, a study has been conducted on an immature type II Kimmeridge clay formation source rock (Dorset, UK), with an initial vitrinite reflectance (VR) of 0.31% Ro and total organic carbon content of 14.4%. Water (hydrous) pyrolysis experiments were conducted on the whole immature source rock, the isolated partially matured bitumen-extracted source rock and the isolated bitumen (bitumen generated and extracted from the initial source rock) and mixtures of the isolated partially matured source rock and bitumen using a 22 ml Hastalloy vessel at 320–420 °C for 7–48 h over a pressure range of 115–500 bar. Hydrocarbon gas yields and the increase in VR were greater for the whole rock experiments compared to the experiments on the isolated partially matured source rock and isolated bitumen (no mineral matter present), as well as the experiments on mixtures of the isolated partially matured isolated source rock and bitumen combined. Hydrocarbon gas yields and VR values were found to decrease at 500 bar compared to 180 bar at 350 °C where the effects of pressure retardation were found to be much more significant for the partially matured source rock maturation and bitumen in isolation than for the whole source rock. At 420 °C, gas generation was not affected by pressure, but VR decreased going from 310 to 450 bar. The results obtained demonstrate that the interplay of inherent mineral matter, reactant phase, source rock/kerogen, bitumen and pressure are key factors in determining the extent of hydrocarbon generation and source rock maturation in geological basins.

14/01892 Geochemical characteristics of biogenic gases in China

Ni, Y. *et al. International Journal of Coal Geology*, 2013, 113, 76–87.

A number of contributions have demonstrated that the stable carbon and hydrogen isotopic compositions together with molecular compositions have a great significance on determination for gas origin and gas generation pathways of biogenic gases. Together with some data from published work, a total of 143 gas samples were compiled from different biogenic gas producing locations in China, to investigate the gas origin and gas generation pathways by the molecular composition, stable carbon and hydrogen isotopes. The results demonstrate that biogenic gases in China are dominated by methane with low level of C_{2+3} (generally less than 0.5%) and low $\delta^{13}C_{CH4}$ values (generally $\leq$ 55‰). The relatively high level of C_{2+3} (up to 11.79%) in the biogenic gases from the Baise and Songliao basins indicates the possible mixture of low-mature thermogenic gases. Biogenic gases from the Jiangzhe coastal area (including Shanghai, Zhejiang, and Jiangsu provinces) and Yingqiong basin have δD_{CH4} values greater than − 190‰, indicating marine salt water depositional environments. However, all other gases have δD_{CH4} values less than − 190‰, possibly indicating a terrestrial freshwater or freshwater to slightly saline water depositional environment. The methanogenic pathway of biogenic gases in China is dominated by biogenic carbonate reduction, though a number of these biogenic gases were generated in a terrestrial freshwater or freshwater to slightly saline water depositional environments. Compared to the bacterial carbonate reduction methanognic pathway in the Luliang basin, gas formation mechanism in the Baoshan basin was more toward bacterial methyl-type fermentation, likely due to the relatively higher geothermal gradient in the Baoshan basin.

14/01893 Permeability prediction of coalbed methane reservoirs during primary depletion

Liu, S. and Harpalani, S. *International Journal of Coal Geology*, 2013, 113, 1–10.

Permeability increase in coalbed methane reservoirs during primary depletion, particularly in the San Juan basin, is a well-accepted phenomenon. It is complex since it is influenced by stress conditions and coal matrix shrinkage associated with gas desorption. Understanding the variations in coal permeability is critical in order to reliably project future gas production, or consider other gas migration issues in the reservoir. Since sorption-induced strain plays a critical role in changing the permeability, typically observed, the theoretical strain model should be incorporated into the permeability prediction models. An effort is made in this paper to couple the recently developed sorption-induced strain model with various permeability models. The model first calculates the theoretical coal matrix shrinkage strain and, using the calculated strain, various commonly used permeability models are applied to two sets of field data. The results of the coupled models show that the agreement between the predicted permeability and that observed in the field is very good. The merit of the coupled models is that it can theoretically predict the permeability with less experimental work, making it a more time efficient and economical technique compared to models used in the past.

14/01894 Production data analysis of unconventional gas wells: review of theory and best practices

Clarkson, C. R. *International Journal of Coal Geology*, 2013, 109–110, 101–146.

Unconventional gas reservoirs, including coalbed methane, tight gas and shale gas, have become a significant source of hydrocarbon supply in North America, and interest in these resource plays has been generated globally. Despite a growing exploitation history, there is still much to be learned about fluid storage and transport properties of these reservoirs. A key task of petroleum engineers and geoscientists is to use historical production (reservoir fluid production rate histories, and cumulative production) for the purposes of (1) reservoir and well stimulation characterization and (2) production forecasting for reserve estimation and development planning. Both of these subtasks fall within the domain of quantitative production data analysis (PDA). PDA can be performed analytically, where physical models are applied to historical production and flowing pressure data to first extract information about the reservoir (i.e. hydrocarbon-in-place, permeability-thickness product) and stimulation (i.e. skin or hydraulic fracture properties) and then generate a forecast using a model that has been 'calibrated' to the dynamic data (i.e. rates and pressures). Analytical production data analysis methods, often referred to as rate-transient analysis (RTA), utilize concepts analogous to pressure-transient analysis for their implementation, and hence have a firm grounding in the physics of fluid storage and flow. Empirical methods, such as decline curve analysis, rely on empirical curve fits to historical production data, and projections to the future. These methods do not rigorously account for dynamic changes in well operating conditions (i.e. flowing pressures), or reservoir or fluid property changes. Quantitative PDA is now routinely applied for conventional reservoirs, where the physics of fluid storage and flow are relatively well-understood. RTA has evolved extensively over the past four decades, and empirical methods are now applied with constraints and 'rules of thumb' developed by researchers with some confidence. For unconventional reservoirs, these techniques continue to evolve according to the improved understanding of the physics of fluid storage and flow. In this paper, the latest techniques for quantitative PDA including type-curve analysis, straight-line (flow-regime) analysis, analytical and numerical simulation and empirical methods are briefly reviewed, specifically addressing their adaptation for coalbed methane and shale gas reservoirs. Simulated and field examples are provided to demonstrate application. It is hoped that this article will serve as practical guide to production analysis for unconventional reservoirs as well as reveal the latest advances in these techniques.

14/01895 Water vapour measurements in natural gas in the presence of ethylene glycol
Løkken, T. V. *Journal of Natural Gas Science and Engineering*, 2013, 12, 13–21.
An investigation of hygrometers for monitoring of water vapour (moisture) in natural gas has been performed, with respect to response on ethylene glycol co-exposure. The tested hygrometers are based on: (1) capacitor sensor, (2) quartz crystal microbalance (QCM), (3) fibre-optic sensor and (4) conversion of water to ethyne, quantified by a gas chromatograph (CaC_2-GC). The moisture concentration level in the test gas was 50 μmol/mol during the experiments, corresponding to a frost point of approximately −48 °C (atmospheric pressure). The experiments were performed in the laboratory, using nitrogen as matrix gas. The QCM hygrometer responded with a downward drift of the frost point readings in the presence of traces of ethylene glycol (0.25 and 0.66 μmol/mol, respectively). The drift increased initially when the ethylene glycol concentration increased, and the frost point readings from the QCM hygrometer decreased close to 5 °C during a total of 20 days of ethylene glycol exposure. The QCM hygrometer seemed to recover slowly from the ethylene glycol exposure, indicated by a decreasing upward drift as soon as the ethylene glycol exposure ended. Both tested capacitor hygrometers responded significantly to ethylene glycol exposure. The responses were not uniform, though, with one performing considerably better than the other one. The experiments also demonstrated the insufficiency of chilled mirror techniques for interpreting water frost points or water dew points, with subsequent moisture concentration calculation, in the presence of ethylene glycol, even at trace amounts. This made the chilled mirror technique totally unsuitable for reference measurements after the introduction of ethylene glycol to the test gas. The fibre-optic sensor hygrometer and the CaC_2-GC hygrometer showed minor response for ethylene glycol. In general the results from this work demonstrate the need for careful evaluation of individual moisture monitoring applications, before choosing a hygrometer. A well-considered strategy for quality control of the moisture monitoring, regardless of the chosen hygrometer, is of utmost importance to establish a moisture monitoring system with high accuracy.

Transport, storage

14/01896 A laterally averaged two-dimensional simulation of unsteady supersaturated total dissolved gas in deep reservoir
Feng, J.-j. *et al. Journal of Hydrodynamics, Ser. B*, 2013, 25, (3), 396–403.
Downstream of dams, elevated levels of total dissolved gas (TDG) may be reached, leading to increased incidences of gas-bubble diseases in fish. The supersaturated TDG dissipates and transports more slowly in reservoirs than in natural rivers because of the greater depth and the lower turbulence, which endangers the fish more seriously. With consideration of the topographical characteristics of a deep reservoir, a laterally averaged two-dimensional unsteady TDG model for deep reservoir is proposed. The dissipation process of the TDG inside the water body and the mass transfer through the free surface are separately modelled with different functions in the model. Hydrodynamics equations are solved coupling with those of water temperature and density. The TDG concentration is calculated based on the density current field. A good agreement is found in the simulation of the Dachaoshan Reservoir between the simulation results and the field data of the hydrodynamics parameters and the TDG distribution in the vertical direction and their unsteady evolution with time. The hydrodynamics parameters, the temperature and the TDG concentration are analysed based on the simulation results. This study demonstrates that the model can be used to predict the evolutions of hydrodynamics parameters, the temperature and the TDG distribution in a deep reservoir with unsteady inflow and outflow. The results can be used in the study of the mitigation measures of the supersaturated TDG.

14/01897 A multidisciplinary study of a natural example of a CO_2 geological reservoir in central Italy
Trippetta, F. *et al. International Journal of Greenhouse Gas Control*, 2013, 12, 72–83.
Storage of CO_2 and, in particular, geological storage is one of the most promising solutions to counteract the continued increase of anthropogenic greenhouse-gas emissions. Here the authors present a multidisciplinary study of a natural CO_2 geologic reservoir where fluid overpressure, measured at 85% of the lithostatic load, is trapped at ~4700 m depth in the northern Apennines of Italy. Deep borehole data and seismic reflection profiles show that the observed CO_2 overpressure: (a) is hosted in dome shaped structures that are the result of the interplay between the compressional and extensional tectonic phases of the area and (b) occurs within dolostones that are sealed by Ca-sulfates (anhydrites) horizons. Field studies on outcropping evaporites, that represent exhumed analogues of the lithologies found at depth in the pressurized reservoir, show dolostones affected by fracturing and faulting and Ca-sulfates characterized by ductile folding without macroscopic fractures. Borehole and laboratory P-wave velocities coincide for anhydrites (6.2–6.3 km/s) but are different for dolostones (6.2–6.3 km/s *in situ* and ~7.2 km/s in the laboratory), confirming the different mode of deformation in the two rock types. Since anhydrites are not dominated by fractures, the very low permeability values, $\sim 10^{-19}$ to $\sim 10^{-22}$ m^2, recorded in laboratory experiments, can also be representative for *in situ* conditions. These data confirm the sealing ability of the anhydrites also for high values of fluid pressure. The integration of these datasets suggests that: (1) tectonics and structural position and (2) lithology and associated mode of deformation, play a key role for channelling and trapping deep-seated CO_2-rich crustal fluids.

14/01898 A new process for well-head gas upgrading
Tunå, P. and Hulteberg, C. *Journal of Natural Gas Science and Engineering*, 2013, 13, 1–6.
As oil prices and environmental concerns are increasing, it is of interest to better use the well-head gas. This light fraction co-produced with petroleum is generally flared and in this paper a method for upgrading and returning the co-product to the petroleum stream is suggested. The method is based on a conversion of the gas to synthesis gas and upgrading this synthesis gas into liquid hydrocarbons. But as the placement of such systems would be remote, the design has been performed using the following criteria. First, the system has to be robust in design and second it has to be self-sustaining in that no additional feedstocks or chemicals are required for its operation and thirdly, the product should be crude oil compatible. In the paper, the system has been outlined, the major unit operations designed and heat and mass balances have been determined. Six cases have been compared, differing in reforming and oxygen generation technology. The comparison has been made on both a technical and production economic premises. In each case the investment cost has been determined and from this, and the calculated produced hydrocarbons, a production cost per barrel has been determined. The production of hydrocarbons well-head gas is a viable route and the production cost for the hydrocarbons vary between $71 and $156 a barrel, with the lower cost being quite attractive with the crude prices of recent years (around $100 a barrel). The production cost is however heavily influenced by the investment cost and the fact that the stranded natural gas is considered free. The production of an alternative, upgraded fuel would be a possibility; this however warrants additional investment in both production equipment and infrastructure.

14/01899 A state-of-the-art review of techno-economic models predicting the costs of CO_2 pipeline transport
Knoope, M. M. J. *et al. International Journal of Greenhouse Gas Control*, 2013, 16, 241–270.
This study aims to provide a systematic overview and comparison of capital and O&M costs models for CO_2 pipelines and booster stations currently available in literature. The findings indicate significantly large cost ranges for the results provided by the different cost models. Two main types of capital cost models for pipeline transport were found in literature, models relating diameter to costs and models relating mass flow to costs. For the nine diameter based models examined, a capital cost range is found of, for instance, 0.8–5.5 M€$_{2010}$/km for a pipeline diameter of 0.8 m and a length of 25 km. For the five mass flow based cost models evaluated in this study, a cost range is found of, for instance, 0.9–2.1 M€$_{2010}$/km for a mass flow of 750 kg/s over 25 km (TRUNK-25). An important additional factor is that all capital costs models for CO_2 pipeline transport, directly or indirectly, depend on the diameter. Therefore, a systematic overview is made of the various equations and parameter used to calculate the diameter. By applying these equations and parameters to a common mass flow, height difference and length result in diameters between 0.59 and 0.91 m for TRUNK-25. The main reason for this range was different assumptions about specific pressure drop and velocity. Combining the range for diameter, mass flow and diameter based cost models gives a capital and levelized cost range which varied by a factor of 10 for a given mass flow and length. The levelized cost range will further increase if the discrepancy in O&M costs is added, for which estimations vary between 4.5 and 75 €/m/year for a pipeline diameter of 0.8 m. On top of this, most cost models underestimate the capital costs of CO_2 pipelines. Only two cost models (namely the models who relate the costs to the weight of the pipeline) take into account the higher material requirements which are typically required for CO_2 pipelines. The other sources use existing onshore natural gas pipelines as the basis for their cost estimations, and thereby underestimating the material costs for CO_2 pipelines. Additionally, most cost models are based on relatively old pipelines constructed in the USA in the 1990s

and early 2000s and do not consider the large increase in material prices in the last several years. Furthermore, key model characteristics are identified for a general cost comparison of CCS with other technologies and a system analysis over time. For a general cost comparison of CCS with other technologies, pipeline cost models with parameters which have physical or economic meaning are the preferred option. These are easy to interpret and can be adjusted to new conditions. A linear cost model is an example of such a model. For a system analysis over time, it is advised to adapt a pipeline cost model related to the weight of the pipeline, which is the only cost model that specifically models thickness of the pipeline and include material prices, to incorporate the effect of impurities and pipeline technology development. For modelling booster station costs, a relation between capacity and costs including some economies of scale seems to be the most appropriate. However, the cost range found in literature is very large, for instance, 3.1–3.6 M€$_{2010}$ for a booster station with a capacity of 1.25 MW$_e$. Therefore, validation of the booster station cost is required before such models are applied in further research.

14/01900 Combined effects of directional compaction, non-Darcy flow and anisotropic swelling on coal seam gas extraction

Wang, J. G. *et al. International Journal of Coal Geology*, 2013, 109–110, 1–14.

The effects of directional compaction, non-Darcy flow and anisotropic swelling on the extraction of natural gas in coal seam reservoirs are important but not well understood so far. This paper investigated these combined effects through a numerical model which fully couples the interactions of coal seam deformation, anisotropic gas flow in fractures, and anisotropic absorption/adsorption of natural gas in coal matrix. In the sorption process, the Langmuir isotherm is extended by including some microstructure information to describe sorption induced anisotropic swelling strain (called anisotropic swelling). The Forchheimer equation is reformulated to consider the non-Darcy effect in directional flows (called non-Darcy flow). A strain ratio of matrix to fractured element is introduced for the directional compaction induced evolution of permeability (called directional compaction). The effect of anisotropic swelling strain is also converted into anisotropic swelling body forces in the mechanical deformation process. This model is verified by the experimental results of single fracture flow under compaction. This verified model is used to quantify the relative importance of directional compaction and matrix swelling through a block model containing a single fracture. It is found that directional compaction of the single fracture can reduce the permeability by 70% and matrix swelling can reduce the permeability by over 30%. This example illustrates the important contribution of matrix swelling to the anisotropy of permeability. This fully-coupled model is applied to a production well in a coal seam gas reservoir to investigate the combined effects of directional compaction, non-Darcy flow and anisotropic swelling on well production rates. It is found that both directional compaction and anisotropic swelling can significantly induce the anisotropy of permeability, forming a skin damaged zone and largely affecting the production rate of natural gas extraction. Directional compaction and anisotropic swelling can significantly accentuate the non-Darcy effect near wellbore for unconventional coal seam gas reservoirs. Thus, the anisotropic evolution of permeability near wellbore cannot be ignorable for the evaluation of production data.

14/01901 Designing learning curves for carbon capture based on chemical absorption according to the minimum work of separation

Rochedo, P. R. R. and Szklo, A. *Applied Energy*, 2013, 108, 383–391.

Carbon capture is one of the most important alternatives for mitigating greenhouse gas emissions in energy facilities. The post-combustion route based on chemical absorption with amine solvents is the most feasible alternative for the short term. However, this route implies in huge energy penalties, mainly related to the solvent regeneration. By defining the minimum work of separation (MWS), this study estimated the minimum energy required to capture the CO_2 emitted by coal-fired thermal power plants. Then, by evaluating solvents and processes and comparing it to the MWS, it proposes the learning model with the best fit for the post-combustion chemical absorption of CO_2. Learning models are based on earnings from experience, which can include the intensity of research and development. In this study, three models are tested: Wright, DeJong and D&L. Findings of the thermochemical analysis indicated a MWS of 0.158 GJ/t for post-combustion. Conventional solvents currently present an energy penalty eight times the MWS. By using the MWS as a constraint, this study found that the D&L provided the best fit to the available data of chemical solvents and absorption plants. The learning rate determined through this model is very similar to the ones found in the literature.

14/01902 Dual layer hollow fiber sorbents for trace H_2S removal from gas streams

Bhandari, D. A. *et al. Chemical Engineering Science*, 2013, 94, 256–264.

Hollow fibre sorbents are pseudo monolithic materials with potential use in various adsorption-based applications. Dual-layer hollow fibre sorbents have the potential to allow thermal regeneration without direct contact of the regeneration fluid with the sorbent particles. This paper considers the application of dual layer hollow fibre sorbents for a case involving trace amounts of H_2S removal from a simulated gas stream and offers a comparison with single-layer hollow fibre sorbents. The effect of spin dope composition and core-layer zeolite loading on the gas flux, H_2S transient sorption capacity and pore structure are also studied. This work can be used as a guide to develop and optimize dual-layer hollow fibre sorbent properties beyond the specific example considered in this paper.

14/01903 Experimental study and techno-economical evaluation of Khangiran sour natural gas condensate desulfurization process

Moaseri, E. *et al. Journal of Natural Gas Science and Engineering*, 2013, 12, 34–42.

There is a serious global concern for removal of different sulfur components from a variety of hydrocarbon products leading to strict regulations to keep sulfur content of various fuels as low as possible. Sour gas condensate production in Khangiran refinery has been tripled in the last 6 years due to the approach of reservoir conditions to the natural gas phase envelope boundary. The significant quantity of sour condensate produced creates several operational and environmental difficulties. To propose a proper process for removal of sulfur species from Khangiran sour condensate, several experiments are performed by considering various scenarios. The oxidative desulfurization process provided best results and is able to decrease the total sulfur content from 8500 ppm to less than 700 ppm by eliminating all hydrogen sulfide and mercaptans and severely reducing other heavy sulfur containing compounds. The odor of the treated condensate was completely improved due to removal of all volatile sulfur components. The preliminary techno-economic evaluation of an industrial scale process is performed based on the experimental results. It is clearly shown that the proposed process is beneficial from both financial and environmental standpoints.

14/01904 Infill well placement optimization in coal bed methane reservoirs using genetic algorithm

Salmachi, A. *et al. Fuel*, 2013, 111, 248–258.

The unprecedented growth of coalbed methane drilling, expensive coalbed water treatment, and low gas rates urge the integration of petroleum engineering and optimization disciplines to meet production goals. An integrated framework is constructed to attain best-obtained optimal locations of infill wells in coalbed methane reservoirs. This framework consists of a flow simulator (ECLIPSE E100), an optimization method (genetic algorithm), and an economic objective function. The objective function is the net present value of the infill project based on an annual discount rate. Best obtained optimal well locations are attained using the integrated framework when net present value is maximized. In this study, a semi synthetic model is constructed based on the Tiffany unit coalbed data in the San Juan basin. The number of infill wells in reservoir resulting in peak production profit is selected as an optimum number of the infill drilling plan. Cost of water treatment and disposal is a key economical parameter which controls infill well locations across the reservoir. When cost of water treatment is low, infill wells are mostly located in virgin section of the reservoir where reservoir pressure is high and fracture porosity is low. Water content in fractures does not play a significant role on infill wells selection when water treatment and disposal is a cheap operation. When cost of water treatment is high, infill wells are mostly located on the transition section between virgin and depleted sections of the reservoir to minimize water production.

14/01905 Investigating the performance of dehydration unit with Coldfinger technology in gas processing plant

Rahimpour, M. R. *et al. Journal of Natural Gas Science and Engineering*, 2013, 12, 1–12.

Natural gas is usually saturated with water that must be removed in order to protect the gas system from corrosion and hydrate formation. Triethylene glycol (TEG) dehydrators are the most common equipment to remove water from the produced gas. TEG regeneration by Coldfinger technology has been recognized as one of the promising processes for dehydrating natural gas. In this work the dehydration unit of the domestic gas processing plant was simulated in the presence of a Coldfinger system. The lack of a Coldfinger unit in steady-state simulation software makes simulation difficult, so, first the Coldfinger was modelled. The predicted results for Coldfinger were compared with plant data. There was a good consistency between them. Then the proposed model was added in the steady-state simulation software. Finally, the result of simulation was used to investigate the influence of

flow rate and temperature of stripping gas and pressure of Coldfinger, on regeneration rate. This research resulted in beneficial information about the performance of the Coldfinger technology.

14/01906 Simulation of gas kick with high H_2S content in deep well

Sun, B.-j. *et al. Journal of Hydrodynamics, Ser. B*, 2013, 25, (2), 264–273.

The phase transition, from a subcritical state to a gaseous state, of the natural gas with high H_2S content and the solubility of the H_2S component in the drilling fluid will make the multiphase flow behaviour very different from the pure natural gas-drilling fluid two-phase flow under the gas kick condition in a deep well. With consideration of the phase transition and the solubility of the H_2S component in the natural gas, a multiphase flow model is established. The simulation analysis results indicate that, for a typical case of a well depth of 4325 m, the density of the 100%-H_2S natural gas can be four times higher than that of the 0%-H_2S natural gas, and the solubility of the 100%-H_2S natural gas is 130 times higher than that of the 0%-H_2S natural gas. These will make the detection of the gas invasion more difficult. While the invasion gas moves up along the wellbore to a certain position, the phase transition and the release of the dissolved gas may cause a rapid volume expansion, increasing the blowout risk. The calculation results also show that the risks of a gas kick can be reduced by increasing the wellhead back pressure.

14/01907 The major sources of gas flaring and air contamination in the natural gas processing plants: a case study

Davoudi, M. *et al. Journal of Natural Gas Science and Engineering*, 2013, 13, 7–19.

Global flaring and venting of natural gas is a significant source of greenhouse gas emissions and airborne pollutants that has proven difficult to mitigate. The impact of such emissions, both on the climate and the environment, makes it inevitable for researchers, environmentalists and policymakers to focus on this issue in recent times. This paper revolves around highlighting potential and critical situations, identifying the proper mitigation and focusing on the sources of flaring and contamination to reduce the generation of wastes from the gas-processing plants of a domestic natural gas field in Iran. The flaring management of four domestic gas processing plants with the total capacity of 252 million m^3 of natural gas per day plays an important role in the environmental pollution reduction. The inventory of emissions lists all the individual sources of air contamination in each gas-processing plant and the quantities of the emissions. The major sources of gas flaring are the regeneration gas coming from the mercaptan removal unit in phase 1, the sweeping gas consumption in the flare network in phases 2 and 3, and the back-up stabilization gas flaring in phases 4 and 5. The adjustment of fuel gas consumption was conducted after the flare network back pressure has been calculated in phases 2 and 3 by a flare net simulator. In order to address the excessive fuel gas network corrosion in phases 6–8, a modification was performed in this gas-processing plant. Chemical de-emulsifier injection allowed the removal of the debris build-up on the rebuilder's tubes of the condensate stabilization column in phases 4 and 5. The recycling regeneration gas of the mercaptan removal unit in phase 1 reduced 55% of the gas flaring in this gas-processing plant.

Economics, business, marketing, policy

14/01908 Access to natural gas storage facilities: strategic and regulation issues

Baranes, E. *et al. Energy Economics*, 2014, 41, 19–32.

This paper analyses the strategic function of gas storage by focusing on how gas-storage decisions have an impact on the competition between gas companies on both spot and downstream markets. Using a two-tier oligopolistic structure, the authors first show that gas storage is actually used strategically even in a symmetric oligopolistic setting along the gas value chain. Storage is then a way to intensify competition on the spot market. Second, the authors analyse the setting where a company has favoured access to storage, for example due to a historical monopolistic position, and analyse this as a leadership situation in the context of third-party access regulation. They then show that this setting compels the leader to adopt a strategic storage decision. This strategy consists of levels of gas stored being greater than supplies available in the downstream market. Such a leader decision is part of a strategy to raise a rival's costs. Furthermore, one can think that optimal regulation of the access to storage facilities would prevent such behaviour. However, especially when storage is not too costly, the authors show that preventing a storage strategy for the leader is not optimal, since the strategy helps to reduce the spot market price.

14/01909 Actual and theoretical gas consumption in Dutch dwellings: what causes the differences?

Majcen, D. *et al. Energy Policy*, 2013, 61, 460–471.

Energy labels in buildings are awarded based on theoretical gas and electricity consumption based on dwelling's physical characteristics. Prior to this research, a large-scale study was conducted in The Netherlands comparing theoretical energy use with data on actual energy use revealing substantial discrepancies. This study uses identical energy label data, supplemented with additional data sources in order to reveal how different parameters influence theoretical and actual consumptions gas and electricity. Analysis is conducted through descriptive statistics and regression analysis. Regression analysis explained far less of the variation in the actual consumption than in the theoretical and has shown that variables such as floor area, ownership type, salary and the value of the house, which predicted a high degree of change in actual gas consumption, were insignificant (ownership, salary, value) or had a minor impact on theoretical consumption (floor area). Since some possibly fundamental variables were unavailable for regression analysis, the authors also conducted a sensitivity study of theoretical gas consumption. It showed that average indoor temperature, ventilation rate and accuracy of *U*-value have a large influence on the theoretical gas consumption; whereas the number of occupants and internal heat load have a rather limited impact.

14/01910 An assessment of the Italian smart gas metering program

Di Castelnuovo, M. and Fumagalli, E. *Energy Policy*, 2013, 60, 714–721.

The introduction of smart metering is one of the core elements in recent European policies targeting environmental sustainability and competitiveness of energy markets. Following the roll-out of smart electricity meters, in 2008 the Italian regulator designed an ambitious deployment programme also for smart gas meters, that was recently modified in both scope and timing. This paper assesses Italy's original and current deployment plans, with a specific focus on the results of its cost–benefit analysis. In light of the evidence derived from the literature, the authors observe that the case for the roll-out of smart gas meters in Italy was not supported by a strong emphasis on energy savings but rather focused on increasing efficiency of the Italian gas market; in this respect, the authors argue that options other than smart gas metering should also be considered. Moreover the Italian cost–benefit analysis, which mostly dealt with the potential cost savings for distributors and suppliers, led to ambiguous results in terms of net present values; thus, an updated assessment would be extremely useful. Finally, in terms of technological choices, this analysis positively evaluates the regulator's recent proposal to consider a dual-fuel solution for the mass market deployment.

14/01911 An optimization model for natural gas supply portfolios of a power generation company

Jirutitijaroen, P. *et al. Applied Energy*, 2013, 107, 1–9.

This paper considers a deregulated electricity market environment where a natural gas-fired generation company can engage in different types of contracts to manage its natural gas supply as well as trade on the electricity market. If the contracts are properly designed, they can protect the company from fluctuations in electricity price and demand, at some cost to the company's expected profit. This reduction in profit can be mitigated by trading on the natural gas and electricity spot markets, but this trading activity may also sometimes result in losses. A stochastic programming model is formulated to capture the hedging decisions made by the company, as well as the interactions between the natural gas and electricity markets. The benefits offered by this approach for profit maximization in a variety of business scenarios, such as the case where the company can hold some amount of gas in storage are studied and presented. It is found that the stochastic model enables the company to optimize the electricity generation schedule and the natural gas consumption, including spot price transactions and gas storage management. Several managerial insights into the natural gas market, natural gas storage, and distribution profit are given.

14/01912 Assessment of energy and economic benefits arising from syngas storage in IGCC power plants

Cocco, D. *et al. Energy*, 2013, 58, 635–643.

This paper aims to evaluate the energy and economic performance of integrated gasification combined cycle (IGCC) power plants equipped with a syngas storage section. Syngas storage enhances operational flexibility of IGCC power plants as a portion of the produced syngas can be stored during periods of low energy demand and used to increase power output during periods of peaking demand, when the produced electrical energy is most valuable and prices are highest. The results of the study show that IGCC systems with syngas storage require a more powerful prime mover and a larger coal gasification section in comparison to base-load IGCC power plants. In the field of duty-cycles of more likely interest (peaking periods of 2–7 h/day and

base/peak power outputs ranging from 0.5 to 0.8), the coal gasification section needs to be enlarged by 5–50% and a fraction from 4% to 30% of the produced syngas needs to be stored. Syngas storage in IGCC power plants leads to a penalty in the overall conversion efficiency (by about 1–6 percentage points in the field of duty-cycles of more practical interest) and higher energy production costs (by about 5–20%) with respect to base-load IGCC power plants.

14/01913 Capital structure in LNG infrastructures and gas pipelines projects: empirical evidences and methodological issues

Pierru, A. *et al. Energy Policy*, 2013, 61, 285–291.

This paper provides new empirical insights on the capital structure of project-financed liquefied natural gas (LNG) infrastructures and gas pipeline projects, by using data relating to projects whose financial close occurred between June 2004 and March 2011. Most results are consistent with the basic view of risk-averse funds suppliers. Especially, the projects located in risky countries and larger projects tend to exhibit lower debt ratios and less-concentrated equity ownerships. In addition, regasification projects appear to have a more diluted equity ownership. Methodological issues raised by the financing of these projects are also examined from a capital-budgeting perspective. In particular, the equity residual method, usually used by industrial practitioners to value these projects, should be adjusted.

14/01914 Determining appliance energy usage with a high-resolution metering system for residential natural gas meters

Tewolde, M. *et al. Applied Energy*, 2013, 108, 363–372.

This paper presents a high-resolution automated meter reading system for residential gas meters, which can be used to record gas consumption for each appliance. The mechanical operation of an industry-standard residential gas meter is characterized, and the internal metering mechanism analysed to develop a system to non-intrusively monitor gas consumption of individual appliances by resolving small amounts of gas usage at the meter. The system can be retrofitted to an existing gas meter with a module that includes a high-resolution encoder to collect gas flow data, and a microprocessor to analyse and classify appliance load profiles. This approach provides a number of attractive features including low cost, easy installation and integration with existing meter reading technologies. This system enables gas utilities to provide real-time feedback to customers on gas usage by appliance.

14/01915 Greenhouse gas emission measurement and economic analysis of Iran natural gas fired power plants

Alavijeh, H. S. *et al. Energy Policy*, 2013, 60, 200–207.

This study attempts to examine the natural gas-fired power plants in Iran. The required data from natural gas fired power plants were gathered during 2008. The characteristics of 32 gas turbine power plants and 20 steam power plants have been measured. Their emission factor values were then compared with the standards of Energy Protection Agency, European Union and the World Bank. Emission factors of gas turbine and steam power plants show that gas turbine power plants have a better performance than steam power plants. For economic analysis, fuel consumption and environmental damages caused by the emitted pollutants are considered as cost functions; and electricity sales revenue are taken as benefit functions. All of these functions have been obtained according to the capacity factor. Total revenue functions show that gas turbine and steam power plants are economically efficient at 98.15% and 90.89% of capacity factor, respectively; this indicates that years of long operating periods of power plants leads to a reduction of optimum capacity factor. The stated method could be implemented to assess the economic status of a country's power plants where as efficient capacity factor close to one means that power plant works in much better condition.

14/01916 Opportunity, challenges and policy choices for China on the development of shale gas

Hu, D. and Xu, S. *Energy Policy*, 2013, 60, 21–26.

With the highest shale gas reserves worldwide and huge need for energy, the Chinese government has introduced many incentives to accelerate the development of shale gas, including subsidies and reduction or waiving of the related fees or taxes. However, the challenges posed by a lack of advanced technologies, environmental protection, a shortage of water in quantity and a knowledge of how to develop a good industry–local community relationship are anticipated in the realization of the predicted golden age of the Chinese shale gas industry. Based on the particular situation and available resources in China, and with reference to the experiences in countries with a developed shale gas industry (such as the USA) and suggestions by the International Energy Agency, recommendations about the choices facing China can be summarized as follows: allowing foreign investors directly to hold exploration and mining rights in shale gas could facilitate the obtainment of advanced technologies; the improvement of the regulatory arrangements related to environmental protection could make developers more responsible; prompting developers to improve their water-use efficiency could help in not worsening the water supply to some extent; and social licence to operate-based mechanism guidance could be helpful in developing a mutual-trust and mutual-benefit relationship between the shale gas industry and the local community.

14/01917 Optimal gas detector placement under uncertainty considering conditional-value-at-risk

Legg, S. W. *et al. Journal of Loss Prevention in the Process Industries*, 2013, 26, (3), 410–417.

A stochastic programming formulation considering conditional-value-at-risk (CVaR) is developed for the optimal placement of gas detectors in petrochemical process facilities. A rigorous gas dispersion simulator, FLACS, is used to generate release scenario data for a real process geometry. This study considers two problem formulations: minimization of expected detection time and minimization of expected detection time subject to a restriction on CVaR across the scenario set. The extensive form of each stochastic program is formulated in Pyomo and solved using CPLEX. Considering all scenarios, the authors compare key values and histograms of detection times for both formulations. Minimizing the mean detection time only can lead to optimal detector placements with a good expected behaviour, but unacceptable worst-case behaviour. The formulations that minimize or constraint CVaR produce sensor placements with significantly better worst-case behaviour and fewer scenarios having high detection times. Considering these results, a strong case for the use of optimal sensor placement using stochastic programming considering CVaR is made for improving safety systems.

14/01918 Projecting EU demand for natural gas to 2030: a meta-analysis

Smith, W. J. *Energy Policy*, 2013, 58, 163–176.

Gas demand projections for the 27 member states of the European Union (EU27), from a variety of sources, are compared. Projected demand varies widely between sources, even when similar rates of economic growth and policy strength are assumed. The divergence is shown to result from differing assumptions concerning future energy intensity, on the one hand, and the future contribution of nuclear power and renewables (RES) to electricity generation on the other. The variation with time of some of these projections is also examined. It is found that the gas demand projected by both the International Energy Agency and the European Commission for 2020 and for 2030 has tended to decrease with each successive projection. This is understandable, since the penetration of RES-E has continued to exceed expectations. However, in an economically depressed, post-Fukushima Europe, estimates of future growth in both RES and nuclear generation may need significant revision. The Energy Efficiency Directive, as agreed by the Council of the European Union and the European Parliament in April 2012, will also have a significant impact on future gas demand, even though the measures incorporated are weaker than the original proposal. The analysis presented here shows that a 'nuclear decline' due to the Fukushima accident is seen to moderate, rather than reverse, projected demand decay. A significant shortfall in projected RES capacity, if it were to occur, constitutes a potential source of additional gas demand. Although the emphasis in this paper is on the EU27 as a whole, consideration is given to the regional heterogeneity of each of these impacts. Hence, although aggregate demand growth for the next decade or two is likely to be moderate or (more probably) negative, local demand growth in some regions may be significant. Ensuring adequate access to these specific regions – via interconnection to their EU27 neighbours, and/or directly from extra-EU sources – will therefore be essential. Hence, implementation of the third energy plan should remain a priority.

14/01919 Shut-in based production optimization of shale-gas systems

Knudsen, B. R. and Foss, B. *Computers & Chemical Engineering*, 2013, 58, 54–67.

This paper presents a novel operational scheme for enhanced utilization of late-life shale multi-well systems. These systems are characterized by a large number of geographically spread wells and pads, where a substantial number of the wells are producing at low erratic rates due to reservoir pressure depletion and well liquid loading. By applying a cyclic shut-in and production strategy, the scheme avoids well liquid loading and optimizes the production from a set of late-life wells at a shared production pad. The scheduling of well shut-ins is formulated as a generalized disjunctive programme (GDP), using a novel shale-gas well and reservoir proxy model. The GDP formulation lends itself both to a complete mixed integer linear programming (MILP) reformulation and reduced size mixed integer non-linear programmingreformulations; a computational study indi-

cates in favour of the MILP formulation. The study includes numerical examples to demonstrate the potential benefit of applying the proposed cyclic scheme compared to a non-optimized approach.

14/01920 The future of the UK gas network

Dodds, P. E. and McDowall, W. *Energy Policy*, 2013, 60, 305–316.

The UK has an extensive natural gas pipeline network supplying 84% of homes. Previous studies of decarbonization pathways using the UK MARKAL energy system model have concluded that the low-pressure gas networks should be mostly abandoned by 2050, yet most of the iron pipes near buildings are currently being replaced early for safety reasons. This study suggests that this programme will not lock-in the use of gas in the long term. The authors examine potential future uses of the gas network in the UK energy system using an improved version of UK MARKAL that introduces a number of decarbonization options for the gas network including bio-methane, hydrogen injection to the natural gas and conversion of the network to deliver hydrogen. The authors conclude that hydrogen conversion is the only gas decarbonization option that might enable the gas networks to continue supplying energy to most buildings in the long term, from a cost-optimal perspective. There is an opportunity for the government to adopt a long-term strategy for the gas distribution networks that either curtails the iron mains replacement programme or alters it to prepare the network for hydrogen conversion; both options could substantially reduce the long-term cost of supplying heat to UK buildings.

14/01921 Using natural gas generation to improve power system efficiency in China

Hu, J. *et al. Energy Policy*, 2013, 60, 116–121.

China's electricity sector faces the challenge of managing cost increases, improving reliability, and reducing its environmental footprint even as operating conditions become more complex due to increasing renewable penetration, growing peak demand, and falling system load factors. Addressing these challenges will require changes in how power generation is planned, priced, and dispatched in China. This is especially true for natural gas generation, which is likely to play an important role in power systems worldwide as a flexible generation resource. Although natural gas is commonly perceived to be economically uncompetitive with coal in China, these perceptions are based on analysis that fails to account for the different roles that natural gas generation plays in power systems: baseload, load following, and peaking generation. This analysis shows that natural gas generation is already cost-effective for meeting peak demand in China, resulting in improved capacity factors and heat rates for coal-fired generators and lower system costs. The largest barrier to using natural gas for peaking generation in China was found to be generation pricing, which could be addressed through modest reforms to support low capacity factor generation.

Derived gaseous fuels

14/01922 A novel reactor configuration for packed bed chemical-looping combustion of syngas

Hamers, H. P. *et al. International Journal of Greenhouse Gas Control*, 2013, 16, 1–12.

This study reports on the application of chemical looping combustion (CLC) in pressurized packed bed reactors using syngas as a fuel. High pressure operation of CLC in a packed bed has a different set of challenges in terms of material properties, cycle and reactor design compared to fluidized bed operation. However, high pressure operation allows the use of inherently more efficient power cycles than low pressure fluidized bed solutions. This paper quantifies the challenges in high pressure operation and introduces a novel reactor concept with which those challenges can be addressed. Continuous cyclic operation of a packed bed CLC system is simulated in a one-dimensional numerical reactor model. Importantly, it is demonstrated that the temperature profiles that can occur in a packed bed reactor as a result of the different process steps do not accumulate, and have a negligible effect on the overall performance of the system. Moreover, it has been shown that an even higher energy efficiency can be achieved by feeding the syngas from the opposite direction during the reduction step (i.e. counter-current operation). Unfortunately, in this configuration mode, more severe temperature fluctuations occur in the reactor exhaust, which is disadvantageous for the operation of a downstream gas turbine. Finally, a novel reactor configuration is introduced in which the desired temperature rise for obtained hot pressured air suitable for a gas turbine is obtained by carrying out the process with two packed bed reactor in series (two-stage CLC). This is shown to be a good alternative to the single bed configuration, and has the added advantage of decreasing the demands on both the oxygen carrier and the reactor materials and design specification.

14/01923 CO_2 reduction to syngas and carbon nanofibres by plasma-assisted *in situ* decomposition of water

Mahammadunniza, S. *et al. International Journal of Greenhouse Gas Control*, 2013, 16, 361–363.

Simultaneous activation of CO_2 and H_2O was carried out in a non-thermal plasma dielectric barrier discharge reactor operated under ambient conditions. The plasma reactor packed with partially reduced NiO/Al_2O_3 catalyst showed better CO_2 conversion than both the unreduced NiO/Al_2O_3 and with plasma (no catalyst), whereas, highest syngas selectivity was observed with unreduced NiO/Al_2O_3. An interesting observation is the formation of carbon nanofibres (CNFs) along with syngas with a reduced NiO catalyst integrated to the plasma, whereas, pure NiO only led to the formation of methane. The reduction of CO_2 by *in situ* formation of hydrogen from water splitting may produce CH_4 and plasma-assisted chemical vapour decomposition of CH_4 may lead to the formation of CNFs.

14/01924 Dimethyl ether synthesis from Victorian brown coal through gasification – current status, and research and development needs

Bhattacharya, S. *et al. Progress in Energy and Combustion Science*, 2013, 39, (6), 577–605.

Victorian brown coal, one of the largest and cheapest energy sources in the world, is currently used in mine-mouth coal-fired power plants. These power plants have low efficiency and high CO_2 emissions. Alternative process paths leading to electricity generation and chemical production can provide more energy efficient and environment friendly applications of brown coal. Synthesis of dimethyl ether (DME) from brown coal is an attractive option because of its environmentally benign properties and wide range of applications. This paper first reviews the current and likely future applications of brown coal. In the latter part of the article emphasis has been given on DME, since it stands out as a suitable option from both environmental and economic point of view. Finally research needs for the development and commercialization of DME production process from brown coal has been identified.

14/01925 Gas production during the pyrolysis and gasification of biological and physico-chemical sludges from oil refinery

Moltó, J. *et al. Journal of Analytical and Applied Pyrolysis*, 2013, 103, 167–172.

Pyrolysis and gasification of two different sludges coming from a Spanish refinery have been performed at different experimental conditions. A physicochemical (PC) and a biological (BIO) sludge have been studied. Runs at different heating rates (approximately 4 and 10 K/s) and with different contact time between gases and decomposed sludge have been performed. In general, the ratio H_2/CO is higher in pyrolytic runs. The highest ratio is obtained in the pyrolysis at low heating rate and parallel flow, using both sludges. The maximum emission of CO, i.e. the worst combustion conditions, is given in the runs where contact time is minimized and at high heating rates.

14/01926 Influence of feedstock composition in fluidised bed co-gasification of mixtures of lignite, bituminous coal and sewage sludge

García, G. *et al. Chemical Engineering Journal*, 2013, 222, 345–352.

Energy recovery from sewage sludge can be achieved by several thermochemical processes, including its co-processing with other fuels. In this work, co-gasification of mixtures of sewage sludge with two types of coal (bituminous and lignite) was performed in a laboratory-scale fluidized bed reactor. The influence of the feedstock composition on key parameters of gasification – such as gas heating value and yield, cold gas efficiency and tar generation – was determined. Whereas some of these results can be explained as the sum of individual contributions of each feedstock component, some synergistic effects were also identified. Among these, the decrease of tar yield and the increase of H_2 and CO in the gas suggest that co-gasification of sewage sludge with certain types of coal may be energetically advantageous and improve the process performance.

14/01927 Interaction of iron–copper mixed metal oxide oxygen carriers with simulated synthesis gas derived from steam gasification of coal

Siriwardane, R. V. *et al. Applied Energy*, 2013, 107, 111–123.

The objective of this work was to prepare supported bimetallic Fe–Cu oxygen carriers and to evaluate their performance for the chemical-looping combustion (CLC) process with simulated synthesis gas derived from steam gasification of coal/air. Ten-cycle CLC tests were conducted with Fe–Cu oxygen carriers in an atmospheric thermogravimetric analyser utilizing simulated synthesis gas derived from the steam gasification of Polish Janina coal and Illinois #6 coal as fuel. The effect of temperature on reaction rates, chemical stability, and oxygen transport capacity were determined. Fractional reduction, fractional oxidation, and global rates of reactions were calculated from the

thermogravimetric analysis (TGA) data. The supports greatly affected reaction performance. Data showed that reaction rates and oxygen capacities were stable during the 10-cycle TGA tests for most Fe–Cu/support oxygen carriers. Bimetallic Fe–Cu/support oxygen carriers showed higher reduction rates than Fe-support oxygen carriers. The carriers containing higher Cu content showed better stabilities and better reduction rates. An increase in temperature from 800 to 900 °C did not have a significant effect on either the oxygen capacity or the reduction rates with synthesis gas derived from Janina coal. Oxidation reaction was significantly faster than reduction reaction for all supported Fe–Cu oxygen carriers. Carriers with higher Cu content had lower oxidation rates. Ten-cycle TGA data indicated that these oxygen carriers had stable performances at 800–900 °C and might be successfully used up to 900 °C for coal CLC reaction in the presence of steam.

14/01928 SiC foam monolith catalyst for pressurized adiabatic methane reforming

Li, C. *et al*. *Applied Energy*, 2013, 107, 297–303.

In this work, an Al_2O_3-coated SiC foam monolith was used as the support of a Ni-based catalyst, which was applied for coupling partial oxidation and steaming reforming of methane to produce syngas or hydrogen. This monolithic catalyst showed excellent structural stability in a 900 h endurance test. Its catalytic activity and stability were also excellent during the first 500 h of the endurance test with a CH_4 conversion (~96%) near thermodynamic equilibrium. Subsequently, it deactivated gradually and its activity was reduced by 7% in the following 400 h. This deactivation is ascribed to deposited carbon that originated from methane cracking in the upper part of the stainless steel reactor. Fresh and used catalyst samples were characterized by XRD, BET, SEM and XRF methods. The results showed that the active coating consisting of Al_2O_3, and the components loaded on it was partially dislodged from the SiC substrate during the reaction, but the loss of Ni loaded on the Al_2O_3 coating was less than the loss of Al_2O_3. This is ascribed to most Ni species being located on the outer surface of the monolithic support, which was more weakly corroded by the reactant flow. The shrinkage of the active coating and the sintering of nickel particles were also observed in the endurance test. Moreover, the SiC foam supported Ni-based monolithic catalyst showed a more homogeneous bed temperature distribution compared with a traditional Ni/Mg–Al spinel catalyst.

14/01929 Syngas fermentation to biofuels: effects of hydrogen partial pressure on hydrogenase efficiency

Skidmore, B. E. *et al*. *Biomass and Bioenergy*, 2013, 55, 156–162.

Producing biofuels from gasified biomass (synthesis gas) via microbial fermentation is currently being pursued as one alternative in biofuels development. In synthesis gas fermentation, reducing equivalents from H_2 oxidation via hydrogenase is important towards directing more carbon towards product formation. In this work, kinetic studies of H_2 utilization via the *Clostridium P11* hydrogenase enzyme were performed to determine the most appropriate model to predict hydrogenase activity as a function of H_2 partial pressure. An important aspect of this work included the proper analysis of electron acceptors used in the kinetic studies. The KH$_2$KH2 model parameter governing the effect of H_2 partial pressure on activity was ~30 kPa (absolute), independent of the type and concentration of electron acceptor. The KH$_2$KH2 value indicates that H_2 partial pressures typically associated with syngas fermentation will result in compromised efficiency of the hydrogenase activity.

LNG

14/01930 Exergy analysis and optimisation of a steam methane pre-reforming system

Dimopoulos, G. G. *et al*. *Energy*, 2013, 58, 17–27.

This paper presents the exergetic analysis and optimization of a steam methane pre-reformer system for marine molten carbonate fuel cells (MCFC) fuelled by liquefied natural gas. The steam methane pre-reformer is a key component of the MCFC, reforming completely higher-chain hydrocarbons and partly methane to hydrogen. The pre-reformer system efficiency improvement is of key importance since it uses up to 10% of the fuel exergy input of the MCFC. First, the authors developed a dynamic mathematical model that describes the physical/chemical behaviour of the pre-reformer system using a generic process modelling framework. Then, they performed exergy analysis and optimized the reformer with respect to its exergetic performance. The developed models and exergy balances were spatially distributed to account for the internal process characteristics, capturing the inter-relation of the local exergy destruction with component design and geometry. An optimization problem was then formulated that minimizes the total irreversibility of the system subject to design, space, technical, and operational constraints. The exergy analysis and optimization for a specific MCFC derived the sources of irreversibility and provided an optimal design of 50% less exergy destruction. The results will serve as a basis for the optimization of the entire MCFC unit.

14/01931 Exergy analysis of combined simultaneous liquid natural gas vaporization and adsorbed natural gas cooling

Roszak, E. A. and Chorowski, M. *Fuel*, 2013, 111, 755–762.

The liquefaction process of natural gas (NG) involves high-energy consumption. Although this energy expenditure is partly offset by benefits in liquefied natural gas (LNG) transportation there is a need of improving the balance of the LNG process chain. Nowadays the cost of liquefaction of LNG oscillates between 0.45 and 0.55 kW h/kg when the thermodynamic minimum is 0.30 kW h/kg (assuming the composition is 100% methane). The proximity of these numbers means that the possibility of improving the liquefaction process is very limited. A different approach to the problem allows LNG as a source of exergy which can be utilized by combining LNG gasification with other processes to be considered. Such solutions can help optimize the economical balance of the overall LNG process chain. The paper proposes a novel idea of coupling the LNG regasification with the filling process of adsorbed natural gas (ANG) tanks. Latent heat of LNG vaporization is directly used for the precooling of the ANG adsorption bed. This enables gas compressors to be avoided and improves the competitiveness of the ANG storage method which is an alternative to compressed natural gas storage and distribution. Exergy analysis presented in the article allows the proposed idea and conventional methods of natural gas regasification to be compared.

14/01932 Experimental study on flow boiling heat transfer of LNG in a vertical smooth tube

Chen, D. and Shi, Y. *Cryogenics*, 2013, 57, 18–25.

An experimental apparatus is set up in this work to study the upward flow boiling heat transfer characteristics of liquefied natural gas (LNG) in vertical smooth tubes with inner diameters of 8 and 14 mm. The experiments were performed at various inlet pressures from 0.3 to 0.7 MPa. The results were obtained over the mass flux range from 16 to 200 kg m^{-2} s^{-1} and heat fluxes ranging from 8.0 to 32 kW m^{-2}. The influences of quality, heat flux and mass flux, tube diameter on the heat transfer characteristic are examined and discussed. The comparisons of the experimental heat transfer coefficients with the predicted values from the existing correlations are analysed. The correlation with an earlier study shows the best accuracy with the root-mean square deviation of 31.7% in comparison with the experimental data.

14/01933 Glass composite vibration isolating structure for the LNG cargo containment system

Choe, J. *et al*. *Composite Structures*, 2013, 107, 469–475.

The primary barrier of the cargo containment system (CCS) for the liquefied natural gas (LNG) carriers is subjected to large impact loads due to the cavitation of LNG. Therefore, the impact loads should be reduced to protect the insulation foam from cracking because the foam has very low fracture toughness at the operating temperature of −163 °C. In this study, a corrugated-plate type vibration isolating structure (VIS) has been developed using glass-fibre reinforced composites to reduce the load transmissibility from the primary barrier to the insulation foam of the CCS at cryogenic temperature. The uniform spring constant characteristic was achieved by optimizing the stacking sequence of the composite laminate and the wavelength of the corrugation. The crack resistance of the VIS against the impact load was measured by the drop weight impact test with respect to the stacking sequence of the glass composite laminate. The specifications of the VIS were obtained by the finite element analysis and experiments. Also, the durability against repetitive impacts on the VIS was investigated.

14/01934 The economic value of LNG in the Korean manufacturing industry

Park, S.-Y. and Yoo, S.-H. *Energy Policy*, 2013, 58, 403–407.

Although liquefied natural gas (LNG) is an important input to industrial production for manufacturing firms, its economic value has been rarely investigated in the literature. This paper attempts to estimate the economic value of LNG in Korea's manufacturing sector by employing the concept of the value of marginal product (VMP). For this, the authors used data on 328 firms using LNG as an input. Two types of production functions (the Cobb–Douglas and trans-log functions) are applied. The result of the specification test indicates that the trans-log function is more appropriate for estimating the data. The output elasticity and VMP of industrial LNG are estimated to be 0.1346 and US$6.22 per m^3, respectively. The results have important implications for various areas of industrial LNG management. For example, any cost–benefit analysis of new projects providing industrial

LNG requires information on the economic value of industrial LNG. In addition, such information is useful for the Korean government's future policies on LNG pricing.

Hydrogen generation and storage

14/01935 A review: feasibility of hydrogen generation from the reaction between aluminum and water for fuel cell applications

Huang, X. *et al. Journal of Power Sources*, 2013, 229, 133–140.

A direct hydrogen fuel cell power system as an alternative of current batteries is promising for portable applications because of its potential better energy and power density. Straight feeding hydrogen, which is generated from a chemical reaction process, to a fuel cell system requires a load–response hydrogen generation rate which is generally not easy to obtain. Hydrogen generation from the reaction between aluminium and water offers a simple way to acquire hydrogen which can be directly fed to a fuel cell power system, however, the oxide film formed on the surface of aluminium particles will generally stop the reaction to proceed. In the present review, metal aluminium activated by various techniques, namely by the addition of alkaline solutions, carbon materials, oxides and by alloying with other elements, are summarized. The effects of the additives on the hydrogen generation characteristics are evaluated. The available hydrogen generators based on the reaction between aluminium and water are discussed and some recommendations for future work are also proposed.

14/01936 Electrochemical synthesis of Ni–S/CeO_2 composite electrodes for hydrogen evolution reaction

Zheng, Z. *et al. Journal of Power Sources*, 2013, 230, 10–14.

Ni–S/CeO_2 electrodes have been prepared by a composite electrodeposition technique using nickel sulfaminate bath containing suspended micro- or nano-sized CeO_2 particles. The composite electrodes exhibit a high activity for the hydrogen evolution reaction (HER) in alkaline solutions, most likely due to the synergistic effects between Ni and CeO_2, as well as the increased surface area of the electrodes upon addition of CeO_2 particles. It is found that the addition of CeO_2 particles can lead to an increase of the sulfur content, resulting in more amorphous structures in the composite coatings. The Ni–S/micro-CeO_2 composite electrode yields a higher HER activity than that measured with Ni–S/nano-CeO_2 electrode, which is 2.2 times higher than that on the Ni–S coating. The relevant discussion was provided to elucidate the promotional roles of CeO_2 particles in the composite electrodeposition process and corresponding HER activity.

14/01937 Evaluation of energy recovery and potential of hydrogen production in Iranian natural gas transmission network

Safarian, S. *et al. Energy Policy*, 2013, 61, 65–77.

In the natural gas transmission network, from supply points to demand nods there are various technological options that include processing, transportation, conversion and gas distribution. Comprehensive analysis of natural gas network requires evaluation of different chains of gas flow through various levels based on economic and environmental criteria subject to technical and operational constraints such as feasibility, operability and reliability of different alternatives. To aid decision-making process in the sector of natural gas, a generic optimization-based model has been developed for assessing long term energy issues related to planning and design of natural gas supply systems. The model is capable of identifying optimal investment strategies and build-up of new capacities of an integrated gas supply system. Evaluation of the potential of energy conservation and hydrogen production in transmission network are also investigated by three energy recovery technologies: turbo expander, organic Rankine cycle and electrolyser. The model has then been applied in studying the development of Iranian natural gas network. The results indicate the utilization of produced hydrogen by electrolyser has considerable impact on minimizing the total cost. The total produced hydrogen of the case study is 1337 million kg, in the period 2011–2030.

14/01938 Hydrogen production from steam reforming of glycerol by Ni–Mg–Al based catalysts in a fixed-bed reactor

Wang, C. *et al. Chemical Engineering Journal*, 2013, 220, 133–142.

About 10 wt% of glycerol can be produced during the conversion of vegetable oils or animal fats into biodiesel fuel by the transesterification process. To make use of glycerol and increase its values, H_2 production from catalytic steam reforming of glycerol by Ni–Mg–Al-based catalysts was evaluated experimentally in a fixed-bed reactor under atmospheric pressure within a temperature range of 450–650 °C. The thermodynamic analysis was conducted by using a non-stoichiometric methodology based on the minimization of Gibbs free energy. The Ni–Mg–Al-based catalysts were synthesized by the co-precipitation method with rising pH technique. The synthesized catalysts were characterized by the elemental analysis, Brunauer–Emmett–Teller, X-ray diffraction and scanning electron microscopy methods. All the metals in the catalyst remained in oxide forms and the catalysts had the specific surface areas from 98.542 to 126.777 m^2/g for different compositions. The results showed that glycerol conversion and H_2 selectivity were increased with increasing temperatures from 450 to 650 °C. The formations of CH_4 and CO in the glycerol steam reforming were almost negligible. Carbon formation in glycerol steam reforming was serious in low temperatures. The catalyst containing NiO of 24.1 wt%, MgO of 26.1 wt% and Al_2O_3 of 49.8 wt% performed appreciable catalytic activity, and the H_2 selectivity was found to be 78.5% and conversion of glycerol was up to 88.0% at 650 °C. The effects of the operating conditions including temperature, the ratio of steam to carbon, glycerol inlet concentration and flow rate of carrier gas on glycerol steam reforming by the optimized catalyst were tested. Based on a kinetic model assuming the power law with a first reaction order, the activation energy and the frequency factor for glycerol steam reforming by the Ni–Mg–Al-based catalysts were calculated.

14/01939 H_2 rich gas production via pressurized fluidized bed gasification of sawdust with in situ CO_2 capture

Han, L. *et al. Applied Energy*, 2013, 109, 36–43.

The continuous increase in energy demand and the growing attention on global warming worldwide have aroused great research interest in a novel near-zero emission energy utilization system which is based on CaO sorption enhanced gasification. This paper presents the experimental results of pressurized CaO sorption enhanced sawdust gasification in a self-design pressurized fluidized bed gasifier, aiming to survey the effects of reaction pressure, CaO to carbon mole ratio (CaO/C), steam to carbon mole ratio (H_2O/C) and reaction temperature (T) on hydrogen (H_2) production under pressurized gasification conditions. The results showed that the pressurized operation not only promoted gasification reactions, but also apparently enhanced CaO carbonation. Within the experimental ranges investigated in this work, H_2 fraction and H_2 yield were both elevated with the increase in reaction pressure, CaO/C, H_2O/C and T. Comparing with previous atmospheric fluidized bed gasification results, pressurized gasification was capable of producing syngas with higher H_2 fraction and lower CO_2 fraction even at lower CaO/C, H_2O/C and T. It was also verified that pressurized operation increased the carbon conversion and cold gas efficiency for CaO sorption enhanced sawdust gasification.

14/01940 Multiple process integrations for broad perspective analysis of fermentative H_2 production from wastewater treatment: technical and environmental considerations

Mohanakrishna, G. and Mohan, S. V. *Applied Energy*, 2013, 107, 244–254.

The functional certainty associated with secondary or tertiary process integration towards enhancing the viability of fermentative biohydrogen (H_2) production from wastewater stabilization was investigated with 11 diverse combinations of dark-fermentation (acidogenic, HA), photo-fermentation (H_P for H_2) and methanogenic (for CH_4) processes. Based on the specificity of individual process, the biocatalyst and the feeding pH were selected and operated at uniform hydraulic retention time (48 h). Individually, H_P operation showed higher H_2 production (4.10 mmol H_2) and yield (16.02 mol H_2/kg COD_R) than of H_A (3.38 mmol H_2, 11.33 mol H_2/kg COD_R) which was found contrary to the observed substrate degradation. Two-stage process integration showed marked improvement in both H_2 production and substrate degradation. Integration of H_P with H_A showed maximum H_2 production while H_A with H_P evidenced maximum H_2 yield. Integration of methanogenic process with H_P documented both higher biogas production and yield. Maximum substrate degradation was evidenced with three-stage sequential integration of dark-fermentation, methanogenic and photo-fermentation processes. Three-stage integration contributed for higher substrate degradation rather than energy generation, especially with HP as the terminal process. Organic flux, energy efficiency and carbon footprint analyses were used to comprehensively delineate the practical consideration of the integrated processes.

14/01941 Performance assessment of solar-based integrated Cu–Cl systems for hydrogen production

Ratlamwala, T. A. H. and Dincer, I. *Solar Energy*, 2013, 95, 345–356.

The present study analyses two integrated systems for hydrogen production, namely, (a) integrated solar heliostat, Cu–Cl cycle and Kalina cycle system and (b) integrated solar heliostat, Cu–Cl cycle, Kalina cycle and electrolyser system. The systems operating parameters, such as, solar radiation intensity, mass fraction of hydrochloric acid and ambient temperature are varied to investigate their effects on hydrogen production rate by both systems, amount of hot water required by the Cu–Cl cycle, amount of water required and

energy and exergy efficiencies of the systems. A comparative study is also carried out to compare the effects of operating parameters on the hydrogen production rate and energy and exergy efficiencies of both the systems. The results show that the system 2 produces 297.7 L/s of hydrogen as compared to 289.4 L/s produced by the system 1 at a solar light intensity of 1200 W/m^2. It is also found that the system 1 performs 2.15% and 3.36% better than the system 2 from energy and exergy perspectives, respectively when solar light intensity is varied. From energy and exergy perspectives, the system 1 performs 1.92% and 2.91% better than the system 2, respectively with variation in the mass fraction of hydrochloric acid. The results show that energy efficiency is not affected by the increase of ambient temperature while the corresponding exergy efficiency increases considerably.

04 BY-PRODUCTS RELATED TO FUELS

14/01942 Co-destruction of organic pollutants in municipal solid waste leachate and dioxins in fly ash under supercritical water using H_2O_2 as oxidant

Zou, D. *et al. Journal of Hazardous Materials*, 2013, 248–249, 177–184.

Supercritical water oxidation, with hydrogen peroxide as oxidant, is applied to the co-disposal of two distinct waste streams: municipal solid waste leachate and incineration fly ash. The chemical oxygen demand (COD) removal efficiency increases rapidly with rising temperature and excess oxygen. Rising residence time from 1 to 2 min has surprisingly little effect. The addition of fly ash accelerates COD conversion markedly and also polychlorinated dibenzo-*p*-dioxins and dibenzofurans (PCDD/Fs, dioxins) in the original fly ash are efficiently destroyed. High-chlorinated PCDD/Fs are more likely to be destroyed than low-chlorinated PCDD/Fs, at all experimental conditions. In addition, PCDDs are much more reactive than PCDFs, since the PCDDs/PCDFs ratio declines from 0.17 to 0.12 as excess oxygen rises from 0% to 300%.

14/01943 Performance improvement and comparison of mass recovery in $CaCl_2$/activated carbon adsorption refrigerator and silica gel/LiCl adsorption chiller driven by low grade waste heat

Lu, Z. S. and Wang, R. Z. *International Journal of Refrigeration*, 2013, 36, (5), 1504–1511.

One $CaCl_2$/activated carbon-ammonia adsorption refrigerator and one silica gel/LiCl-methanol chiller was designed and tested. The comparison of performance improvement of mass recovery process on the two adsorption systems was studied. The results show that the coefficient of performance (COP) and specific of cooling power (SCP) can be improved by 15.4% and 10.5% by mass recovery process in silica gel/LiCl-methanol chiller, while they can be improved by 53.8% and 51.5% in $CaCl_2$/activated carbon–ammonia refrigerator, because the latter has larger pressure difference between the hot and cold bed. Both the $CaCl_2$/activated carbon–ammonia refrigerator and the silica gel/LiCl–methanol chiller can provide continuous and stable cooling capacity. Under nominal working condition, the evaporator temperature, COP and SCP can reach −21 °C, 0.26 and 474 W kg^{-1} in $CaCl_2$/activated carbon–ammonia refrigerator, and they are 15 °C, 0.41 and 244 W kg^{-1} in the silica gel/LiCl–methanol chiller.

14/01944 Performance of coal fly-ash based oxygen carrier for the chemical looping combustion of synthesis gas

Aisyah, L. *et al. Applied Energy*, 2013, 109, 44–50.

The performance of coal fly-ash-based oxygen carriers for chemical looping combustion of synthesis gas has been investigated using both a thermogravimetric analyser and a packed bed reactor. Oxygen carriers with 50 wt% active metal compounds, including copper, nickel and iron oxides, supported on coal fly-ash were synthesized using the deposition–precipitation method. Copper oxide and nickel oxide supported on fly-ash showed high oxygen transfer efficiency and oxygen carrying capacity at 800 °C. The fly-ash-based nickel oxide was effective in reforming hydrocarbons and for the conversion of carbon dioxide into carbon monoxide; a nickel complex with silicate was identified as a minor phase following the reduction reaction. The fly-ash-based iron oxide showed various reduction steps and resulted in an extended reduction time. The carbon emission at the oxidation stage was avoided by reducing the length of the exposure to the reduction gas.

14/01945 Production of low-tar producer gas from air gasification of mixed plastic waste in a two-stage gasifier using olivine combined with activated carbon

Cho, M.-H. *et al. Energy*, 2013, 58, 688–694.

A fraction of mixed plastic waste was gasified using olivine as a bed material and activated carbon as a tar-cracking additive in a two-stage gasifier. The effects of the amount of activated carbon, the use of an activated carbon filter, and the removal of an electrostatic precipitator from the process on the gas composition and tar amount generated were investigated. The effects of the equivalence ratio, the type of distributor, the use of steam and the use of a wire mesh basket for activated carbon on the coke removal were also examined. As a result, H_2 concentrations of around 307tsp;vol% were obtained with 1500 g of activated carbon. The tar removal efficiency was maximized at about 98% with the application of 1500 g of activated carbon and steam. The lower heating values of the producer gases obtained with the two additives at equivalence ratios of about 0.31 were in the range of 5.3–6.2 MJ/N m^3.

14/01946 Reactive adsorption of SO_2 on activated carbons with deposited iron nanoparticles

Arcibar-Orozco, J. A. *et al. Journal of Hazardous Materials*, 2013, 246–247, 300–309.

The effect of iron particle size anchored on the surface of commercial activated carbon on the removal of SO_2 from a gas phase was studied. Nanosize iron particles were deposited using forced hydrolysis of $FeCl_3$ with or without H_3PO_4 as a capping agent. Dynamic adsorption experiments were carried out on either dry or pre-humidified materials and the adsorption capacities were calculated. The surface of the initial and exhausted materials was extensively characterized by microscopic, porosity, thermogravimetric and surface chemistry. The results indicate that the SO_2 adsorption capacity increased two and half times after the prehumidification process owing to the formation of H_2SO_4 in the porous system. Iron species enhance the SO_2 adsorption capacity only when very small nanoparticles are deposited on the pore walls as a thin layer. Large iron nanoparticles block the ultramicropores decreasing the accessibility of the active sites and consuming oxygen that rest adsorption centres for SO_2 molecules. Iron nanoparticles of about 3–4 nm provide highly dispersed adsorption sites for SO_2 molecules and thus increase the adsorption capacity of about 80%. $Fe_2(SO_4)_3$ was detected on the surface of exhausted samples.

14/01947 Removal of As(V) from aqueous solution by activated carbon-based hybrid adsorbents: impact of experimental conditions

Tuna, A. Ö. A. *et al. Chemical Engineering Journal*, 2013, 223, 116–128.

In this study, apricot stone based activated carbon (IAC) was modified with iron (oxy-hydr)oxides to produce effective hybrid adsorbents for arsenic removal from aqueous medium. For this purpose, Fe^{2+} loaded activated carbon (IAC-Fe(II)) and Fe^{3+} loaded activated carbon (IAC-Fe(III)) were produced by precipitation method. As(V) adsorption on each adsorbents was investigated at three levels of pH (3.0, 5.0 and 7.0), initial As(V) concentration (0.5, 4.5 and 8.5 mg L^{-1}) and temperature (298, 318 and 338 K). As(V) adsorption capacities of IAC, IAC-Fe(II) and IAC-Fe(III) were found to be 0.034, 2.023 and 3.009 mg g^{-1}, which represented 15.00%, 98.34%, and 99.05% As(V) removal efficiency, respectively. As(V) adsorption kinetics of hybrid adsorbents were investigated and it was found that IAC-Fe(III) required less contact time than IAC-Fe(II). Thermodynamic parameters such as Gibbs free energy (ΔG°), entropy (ΔS°) and enthalpy (ΔH°) were calculated from experimental isotherm at different temperatures. The value of ΔH° for arsenate adsorption on IAC-Fe(II) was positive that indicates endothermic nature of the adsorption process. On the other hand, IAC-Fe(III) had negative value of ΔH° that indicates exothermic nature of arsenate adsorption. The equilibrium data for both hybrid adsorbents fitted well to Freundlich and Dubinin–Radushkevich. The As(V) adsorption on hybrid adsorbents had high values of correlation coefficient (R^2) and low values of chi-square (χ^2) for all adsorption isotherm model except Langmuir isotherm, indicate that adsorption of As(V) on hybrid adsorbents takes place on multi-layer.

14/01948 Study on the nonylphenol removal from aqueous solution using magnetic molecularly imprinted polymers based on fly-ash-cenospheres

Pan, J. *et al. Chemical Engineering Journal*, 2013, 223, 824–832.

Fly-ash cenospheres/Fe_3O_4 magnetic particles (MFACs) were firstly achieved by co-precipitation technique. After endowing with reactive vinyl groups onto the surface of MFACs, magnetic molecularly imprinted polymers (MMIPs) based on the modified MFACs were further prepared by suspension polymerization. The MMIPs were characterized, and the results indicated that spherical MMIPs exhibited superparamagnetic property ($M_s = 20.99$ emu g^{-1}), magnetic stability (at the pH = 6.0), thermal stability (<100 °C) and composed of imprinted layer. Batch mode adsorption experiments were carried out to investigate the specific adsorption equilibrium, kinetics and selective recognition. The initial pH = 6.0 was the optimal condition, and the hydrogen bond interaction may be the main recognition mechanism. The kinetic properties of MMIPs were well described by

the pseudo-second-order equation, indicating chemical process could be the rate-limiting step in the adsorption process for nonylphenol. The adsorption equilibrium of nonylphenol using MMIPs was better modelled by the Langmuir isotherm equation, and the monolayer adsorption capacity of MMIPs at 298 K was 434.8 mg g^{-1}. The selectivity results showed that MMIPs had the specific adsorption for nonylphenol molecules, and the recognition process may be related to the size, structure and functional group of the template molecules.

05 NUCLEAR FUELS

Scientific, technical

14/01949 Abundant thorium as an alternative nuclear fuel: important waste disposal and weapon proliferation advantages

Schaffer, M. B. *Energy Policy*, 2013, 60, 4–12.

It has long been known that thorium-232 is a fertile radioactive material that can produce energy in nuclear reactors for conversion to electricity. Thorium-232 is well suited to a variety of reactor types including molten fluoride salt designs, heavy-water CANDU configurations, and helium-cooled TRISO-fuelled systems. Among contentious commercial nuclear power issues are the questions of what to do with long-lived radioactive waste and how to minimize weapon proliferation dangers. The substitution of thorium for uranium as fuel in nuclear reactors has significant potential for minimizing both problems. Thorium is three times more abundant in nature than uranium. Whereas uranium has to be imported, there is enough thorium in the USA alone to provide adequate grid power for many centuries. A well-designed thorium reactor could produce electricity less expensively than a next-generation coal-fired plant or a current-generation uranium-fuelled nuclear reactor. Importantly, thorium reactors produce substantially less long-lived radioactive waste than uranium reactors. Thorium-fuelled reactors with molten salt configurations and very high temperature thorium-based TRISO-fuelled reactors are both recommended for priority generation IV funding in the 2030 time frame.

14/01950 Hydromechanical modelling of an excavation in an underground research laboratory with an elastoviscoplastic behaviour law and regularization by second gradient of dilation

Plassart, R. *et al. International Journal of Rock Mechanics and Mining Sciences*, 2013, 58, 23–33.

In the context of nuclear waste disposals, this paper deals with hydromechanical modelling in saturated conditions in deep geological formation, using a specific elastoviscoplastic model hereafter called the L&K model. While classical Biot's framework is followed for the hydromechanical coupling, the mechanical L&K model offers a coupling between instantaneous and delayed behaviour and a variation of dilation often related to softening. These volumetric strains are especially highlighted in coupled hydromechanical conditions. In order to avoid mesh dependency and numerical localized solutions, this type of modelling needs the use of a regularization method which is here referred to as the second gradient dilation model. After describing the numeric tools, the authors use them for simulating a gallery of the underground research laboratory of Bure. The approach is validated by the good general agreement found between numeric results and *in situ* measures for both hydraulic pressure and displacement.

14/01951 Mitigation of effects of pulsed heat load from fusion devices on helium refrigerator: a novel technique using vapor compression cycle

Dutta, R. *et al. International Journal of Refrigeration*, 2013, 36, (6), 1776–1789.

Helium refrigerators used in fusion devices are subjected to pulsed heat load. Immediate effect of such load is high fluctuation of mass flow rate at the return stream. A novel technique using vapour compression cycle at the cold end of helium refrigerators has been proposed to mitigate this flow fluctuation. The concept behind the proposed scheme is to re-liquefy excess return stream during high heat load condition and store. During low heat load condition, mitigation is obtained by increasing vapour fraction after expansion in Joule–Thomson valves by increasing inlet temperature of these valves. Dynamic simulation of a plant modified with vapour compression cycle has been performed and it has been found that approximately 70% and 96% mitigation of flow fluctuation during high and low heat load respectively, can be achieved. Criteria of selection and technical feasibility of critical equipment for implementation of the concept have also been discussed.

14/01952 Morphology of uranium electrodeposits on cathode in electrorefining process: a phase-field simulation

Shibuta, Y. *et al. Journal of Nuclear Materials*, 2013, 436, (1–3), 61–67.

Morphology of uranium electrodeposits on cathode with respect to applied voltage, zirconium concentration in the molten salt and the size of primary deposit during pyroprocessing is systematically investigated by the phase-field simulation. It is found that there is a threshold zirconium concentration in the molten salt demarcating planar and cellular/needle-like electrodeposits, which agrees with experimental results. In addition, the effect of size of primary deposits on the morphology of electrodeposits is examined. It is then confirmed that cellular/needle-like electrodeposits are formed from large primary deposits at all applied voltages considered, whereas both the planar and cellular/needle-like electrodeposits are formed from the primary deposits of 10 μm and less.

14/01953 Photothermal microscopy applied to the characterization of nuclear fuel pellets

Escola, F. Z. *et al. Journal of Nuclear Materials*, 2013, 435, (1–3), 17–24.

The photothermal photodeflection technique is shown to provide information on the homogeneity of fuel pellets, pore distribution, clustering detection of pure urania and gadolinea and to provide a two-dimensional mapping of the thermal diffusivity correlated to the composition of the interdiffused Gadolinium and Uranium oxide. Histograms of the thermal diffusivity distribution become a reliable quantitative way of quantifying the degree of homogeneity and the width of the histogram can be used as a direct measure of the homogeneity. These quantitative measures of the homogeneity of the samples at microscopic levels provides a protocol that can be used as a reliable specification and quality control method for nuclear fuels, substituting with a single test a battery of expensive, time consuming and operator-dependent techniques.

14/01954 Recrystallization and fission-gas-bubble swelling of U–Mo fuel

Kim, Y. S. *et al. Journal of Nuclear Materials*, 2013, 436, (1–3), 14–22.

At high burn-up, U–Mo fuel exhibits some form of recrystallization, by which fuel grains are subdivided. The effect of grain subdivision is to effectively enhance fission gas bubble (FGB) swelling due to increased grain boundaries. Inter-granular FGB swelling, i.e. FGB formation and growth at the grain boundaries, is much larger than the intra-granular FGB swelling. Recrystallized fuel volume fractions of U–Mo fuels irradiated to fission densities reaching 5.7×10^{21} f/cm^3 were measured. Analytical expressions of recrystallization kinetics of U–Mo fuel during irradiation have been developed through the usage of the Avrami equation, a phenomenological equation which is also used to describe similar typical transformation reactions, such as new phase formation. The study presents a novel FGB swelling model of U–Mo fuel that is expressed in terms of Mo content, extent of cold work (fuel powder fabrication method), and fission density.

14/01955 Reliability analysis of stainless steel piping using a single stress corrosion cracking damage parameter

Guedri, A. *International Journal of Pressure Vessels and Piping*, 2013, 111–112, 1–11.

This paper presents the results of an investigation that combines standard methods of fracture mechanics, empirical correlations of stress-corrosion cracking and probabilistic methods to provide an assessment of intergranular stress corrosion cracking (IGSCC) of stainless-steel piping. This is done by simulating the cracking of stainless-steel piping under IGSCC conditions using the general methodology recommended in the modified computer program 'Piping Reliability Analysis Including Seismic Events', and by characterizing IGSCC using a single damage parameter. Good correlation between the pipe end-life probability of leak and the damage values were found. These correlations were later used to generalize this probabilistic fracture model. Also, the probability of detection curves and the benefits of in-service inspection in order to reduce the probability of leak for nuclear piping systems subjected to IGSCC were discussed for several pipe sizes. It was found that greater benefits could be gained from inspections for the large pipe as compared to the small pipe sizes. Also, the results indicate that the use of a better inspection procedure can be more effective than a 10-fold increase in the number of inspections of inferior quality.

14/01956 Shifting strategies and precarious progress: nuclear waste management in Canada

Ramana, M. V. *Energy Policy*, 2013, 61, 196–206.

Canada has a lengthy history of trying to find ways of dealing with radioactive spent fuel and nuclear waste from its nuclear reactors. In the past decade, Canada has taken major strides towards this goal by evolving a process through which a site for a geological repository to sequester nuclear waste is to be selected. The Canadian Nuclear Waste Management Organization (NWMO) is in the early stages of the process of finding a community that is willing to host such a repository. Differences between the broad principles underlying siting and the processes for actually selecting the site have emerged as the NWMO proceeds with engaging local governments and specific communities. These differences and other conflicts, especially over new nuclear reactor construction, might pose hurdles in the path of successfully setting up a repository.

14/01957 Study on laser welding of fuel clad tubes and end plugs made of modified 9Cr–1Mo steel for metallic fuel of fast breeder reactors

Harinath, Y. V. *et al. Journal of Nuclear Materials*, 2013, 435, (1–3), 32–40.

A procedure for pulsed laser beam welding (PLBW) has been developed for fabrication of fuel pins made of modified 9Cr–1Mo steel for metallic fuel proposed to be used in future in India's fast breeder reactor programme. Initial welding trials of the samples were carried out with different average power using Nd-YAG based PLBW process. After analysing the welds, average power for the weld was optimized for the required depth of penetration and weld quality. Subsequently, keeping the average power constant, the effect of various other welding parameters, such as laser peak power, pulse frequency, pulse duration and energy per pulse on weld joint integrity were studied and a procedure that would ensure welds of acceptable quality with required depth of penetration, minimum size of fusion zone and heat-affected zone were finalized. This procedure is also found to reduce the volume fraction delta-ferrite in the fusion zone.

14/01958 Thermal–hydraulic analysis of the cool-down for the ITER magnets

Peng, N. *et al. Cryogenics*, 2013, 57, 45–49.

A three-dimensional time-dependent cool-down simulation for the international thermonuclear experimental reactor (ITER) magnet system has been performed. The total cold mass of the magnet system is about 10,130 ton, namely 18 toroidal field winding packs and their mechanical cases, six poloidal field coils, central solenoid and a set of correction coils. All ITER coils are made from cable-in-conduit conductor superconductors. This paper presents the simplified flow scheme of the magnet system and the simulation models. The simulated temperature evolutions of entire processes of cool-down are showed. The functions of the inlet temperature for cool-down are summarized. The simulation results indicate that it is possible to cool down the entire ITER magnet system to 6 K within 750 h.

Economics, policy, supplies, forecasts

14/01959 A case study of economic incentives and local citizens' attitudes toward hosting a nuclear power plant in Japan: impacts of the Fukushima accident

Kato, T. *et al. Energy Policy*, 2013, 59, 808–818.

The attitude of local communities near a nuclear power plant (NPP) is a key factor in nuclear policy decision making in Japan. This case study compared local citizens' attitudes in 2010 and 2011 toward the benefits and drawbacks of hosting Kashiwazaki–Kariwa NPP. The Fukushima accident occurred in this period. After the accident, benefit recognition of utility bill refunds clearly declined, while that of public facilities did not, suggesting the influence of a bribery effect. The negative shift of attitudes about hosting the NPP after the accident was more modest in Kariwa village, which saw a large expansion of social welfare programmes, than in the other two areas, which lacked such a budget expansion. Policy implications of these results regarding the provision of economic incentives in NPP host areas after the Fukushima accident were discussed.

14/01960 A lead for transvaluation of global nuclear energy research and funded projects in Japan

Kiriyama, E. *et al. Applied Energy*, 2013, 109, 145–153.

The decision-making process that precedes the introduction of a new energy system should strive for a balance among human security, environmental safeguards, energy security, proliferation risk, economic risks, etc. For nuclear energy, the Fukushima Daiichi nuclear disaster has brought forth a strong need for transvaluation of the present technology. The authors analysed bibliographic records of publications in nuclear science and technology to illustrate an overview and trends in nuclear energy technology and related fields by using citation network analysis. They also analysed funding data and keywords assigned for each project by co-occurrence network analysis. This research integrates citation network analysis and bibliometric keyword analysis to compare the global trends in nuclear energy research and characteristics of research conducted at universities and institutes in Japan. The authors show that the Chernobyl accident had only a limited influence on basic research. The results of papers are dispersed in diverse areas of nuclear energy technology research, and the results of KAKEN projects in Japan are highly influenced by national energy policy with a focus on nuclear fuel cycle for energy security, although KAKEN allows much freedom in the selection of research projects to academic community.

14/01961 A scenario-based modeling approach for emergency evacuation management and risk analysis under multiple uncertainties

Lv, Y. *et al. Journal of Hazardous Materials*, 2013, 246–247, 234–244.

Nuclear emergency evacuation is important to prevent radioactive harms by hazardous materials and to limit the accidents' consequences; however, uncertainties are involved in the components and processes of such a management system. In the study, an interval-parameter joint-probabilistic integer programming (IJIP) method is developed for emergency evacuation management under uncertainties. Optimization techniques of interval-parameter programming and joint-probabilistic constrained programming are incorporated into an integer linear programming framework, so that the approach can deal with uncertainties expressed as joint probability and interval values. The IJIP method can schedule the optimal routes to guarantee the maximum population evacuated away from the effected zone during a finite time. Furthermore, it can also facilitate post optimization analysis to enhance robustness in controlling system violation risk imposed on the joint-probabilistic constraints. The developed method has been applied to a case study of nuclear emergency management; meanwhile, a number of scenarios under different system conditions have been analysed. It is indicated that the solutions are useful for evacuation management practices. The result of the IJIP method can not only help to raise the capability of disaster responses in a systematic manner, but also provide an insight into complex relationships among evacuation planning, resources utilizations, policy requirements and system risks.

14/01962 Acceptance of nuclear power: the Fukushima effect

Siegrist, M. and Visschers, V. H. M. *Energy Policy*, 2013, 59, 112–119.

Utilizing a longitudinal study design, the impact of the 2011 accident in Fukushima on acceptance of nuclear power and the evaluation of several scenarios with different percentages of nuclear power were examined. Mail surveys were conducted in the German-speaking part of Switzerland. The first survey took place before the accident in Fukushima (autumn 2010), the second survey immediately after the accident (March 2011), and the third survey half a year after the accident (October 2011). A sample of 463 persons participated in all three surveys. The accident had a negative impact on the acceptance of nuclear power. The mean change was moderate, and high correlations between the measurement points were observed. Overall, participants thus showed rather stable attitudes towards nuclear power across the three measurement waves. Results of the present study demonstrate the importance of prior beliefs and attitudes for the interpretation of an accident. The evaluation of the various scenarios was strongly influenced by participants' pre-Fukushima attitudes towards nuclear power.

14/01963 Belgian nuclear power life extension and fuss about nuclear rents

Verbruggen, A. *Energy Policy*, 2013, 60, 91–97.

Nuclear decision-making is embedded in slowly evolving political, economic and financial institutions. Belgium houses extended nuclear activities, mostly under French control, for example: SUEZ-GDF and EDF own all Belgian nuclear power plants. But a 2003 law mandates the closure of Belgium's nuclear power plants at a service age of 40 years; only *force majeure* could lift the strict obligation. Opposition to the law argued with climate change danger, financial losses, and loss-of-load risks. The financial issue got interwoven with a fuzzy debate on the definition, height and appropriation of 'nuclear rents'. As plausible hypothesis is adopted: the prospected transfer of hundreds millions of euros from power companies to the public interest will create public support for life extension. But the nuclear rents discussion had faded in July 2012 when the Belgian government admitted a 10-year life extension for TIHANGE I (962 MW) and imposed the closure of the 2×433 MW DOEL I and II. Loss-of-load risk was the government's only public argument. The opacity of the decision process and its '50–50' outcome do not allow proper testing of the hypothesis. The case illustrates that politicians cannot bind their followers except through the deployment of alternative power sources.

14/01964 EU Carbowaste project: development of a toolbox for graphite waste management
Metcalfe, M. P. *et al. Journal of Nuclear Materials*, 2013, 436, (1–3), 158–166.
A 4-year collaborative European Union (EU) project, 'Treatment and Disposal of Irradiated Graphite and Other Carbonaceous Waste (Carbowaste)', was launched in May 2008 under the seventh EURATOM framework programme. The aim of the project is to develop best practices in the retrieval, treatment and disposal of irradiated graphite, addressing both existing legacy waste as well as waste from graphite-based nuclear fuel resulting from a new generation of nuclear reactors. This paper covers the activities led by the UK's National Nuclear Laboratory in partnership with the UK's Nuclear Decommissioning Authority in the first year of the project, which includes the lead role in the compilation of a review volume on the extent of irradiated graphite waste globally and the approaches being taken to manage it. An overview is also provided of modelling activities in the second year of the project: the application of modelling techniques to the prediction of radiological inventories, to the radiological impact of C-14 and Cl-36 releases on the biosphere and to the decommissioning of Magnox reactor cores.

14/01965 Impact of the German nuclear phase-out on Europe's electricity generation – a comprehensive study
Bruninx, K. *et al. Energy Policy*, 2013, 60, 251–261.
The combination of the ambitious German greenhouse gas reduction goals in the power sector and the nuclear phase-out raises many questions concerning the operational security of the German electricity generation system. This paper focuses on the technical feasibility (electricity generation and transmission) and CO_2-impact of the German nuclear phase-out on the short term (2012–2022). A detailed electricity generation simulation model is employed, including the German transmission grid and its international connections. A range of different conventional and renewable energy sources (RES) scenarios is considered. Results are presented for the change in generation mix, on the flows on the transmission network and on operational reliability issues. The scenario analysis shows that nuclear generation will be replaced mainly by coal- and lignite-based generation. This increases the CO_2-intensity of the German electricity sector. Furthermore, the results indicate that the German electricity export will decrease and under certain circumstances, the system no longer becomes feasible. Keeping some nuclear power plants online, would mitigate these effects. The amount of electricity generated from RES is shown to be the main driver for grid congestion.

14/01966 Japan's post-Fukushima reconstruction: a case study for implementation of sustainable energy technologies
Nesheiwat, J. and Cross, J. S. *Energy Policy*, 2013, 60, 509–519.
Following World War II, Japan developed into an economic powerhouse and a model of energy efficiency among developed countries. This lasted more than 65 years until the earthquake in north-eastern Japan and tsunami-induced nuclear crisis of March 2011 brought Japan to an existential crossroads. Instead of implementing its plans to increase nuclear power generation capacity from 30% to 50%, Japan shut all 54 nuclear reactors for safety checks and stress checks (two have since been restarted), resulting in reduced power generation during the summer of 2012. The reconstruction of north-eastern Japan approaches at a time when the world is grappling with a transition to sustainable energy technologies – one that will require substantial investment but one that would result in fundamental changes in infrastructure and energy efficiency. Certain reconstruction methods can be inappropriate in the social, cultural and climatic context of disaster affected areas. Thus, how can practitioners employ sustainable reconstructions which better respond to local housing needs and availability of natural energy resources without a framework in place? This paper aims at sensitizing policy-makers and stakeholders involved in post disaster reconstruction by recognizing advantages of deploying sustainable energy technologies, to reduce dependence of vulnerable communities on external markets.

14/01967 The cross-section of returns, benchmark model parameters, and idiosyncratic volatility of nuclear energy firms after Fukushima Daiichi
Lopatta, K. and Kaspereit, T. *Energy Economics*, 2014, 41, 125–136.
This study analyses how the stock market returns, the factor loadings from the Carhart four-factor model and the idiosyncratic volatility of shares in energy firms, have been affected by the Fukushima nuclear accident. Unlike existing studies, which provide evidence of a wealth transfer from nuclear to renewable energy firms for specific countries, the authors use an international sample and investigate whether changes in the regulatory environment and the firm-specific commitment to nuclear and renewable energies correlate with the capital market's reactions to the Fukushima Daiichi accident. The findings suggest that the more a firm relies on nuclear power, the more its share price declined after the accident. A commitment to renewable energies does not prevent declines in share prices but significantly helps to reduce the increase in market beta that is associated with this event. Nuclear energy firms domiciled in countries with a higher number of regulatory interventions that were triggered by the catastrophe have lower abnormal returns than those that are domiciled elsewhere. However, as a cross-sectional analysis reveals, a stronger commitment to nuclear power is the main driver for negative stock market returns. Furthermore, nuclear energy firms domiciled in countries with stronger regulatory shifts away from nuclear energy experience significant increases in market beta and the book-to-market equity factor loading according to the Carhart four-factor model. It can be concluded that capital market participants are able to differentiate between the affectedness of firms with respect to their product portfolio. Energy firms could prevent increases in market beta due to catastrophes such as the Fukushima Daiichi accident by shifting some of their energy production from nuclear to renewable or other sources.

14/01968 The importance of nuclear energy for the expansion of Brazil's electricity grid
dos Santos, R. L. P. *et al. Energy Policy*, 2013, 60, 284–289.
This article analyses the thermal energy options available in the Brazil to support the expansion of the country's electricity grid capacity. Brazil's electricity mix consists primarily of renewable sources of energy and this configuration will be maintained throughout the twenty-first century. However, grid expansion can no longer benefit from hydroelectric power plants with large reservoirs leading to a greater participation of thermal power plants. Among the thermal sources available in the country, nuclear power has important comparative advantages. Recognizing these benefits, the Brazilian government has established that expanding electricity grid capacity will amount to up to 8000 MW through nuclear energy by 2030. The use of nuclear technology for electricity generation has historically been a controversial issue worldwide and some countries have decided to review their nuclear programs in the aftermath of the 2011 Fukushima nuclear accident. This article shows that increasing the participation of nuclear energy in Brazil's electricity grid will provide important benefits for the country by ensuring energy security, keeping Brazil's electricity mix as one of the cleanest in the world, securing electricity grid reliability and safety and reducing operating costs.

06 ELECTRICAL POWER SUPPLY AND UTILIZATION

Scientific, technical

14/01969 A method for predicting city-wide electricity gains from photovoltaic panels based on LiDAR and GIS data combined with hourly Daysim simulations
Jakubiec, J. A. and Reinhart, C. F. *Solar Energy*, 2013, 93, 127–143.
This study presents, demonstrates and validates a method for predicting city-wide electricity gains from photovoltaic (PV) panels based on detailed three-dimensional urban massing models combined with Daysim-based hourly irradiation simulations, typical meteorological year climactic data and hourly calculated rooftop temperatures. The resulting data can be combined with online mapping technologies and search engines as well as a financial module that provides building owners interested in installing a PV system on their rooftop with meaningful data regarding spatial placement, system size, installation costs and financial payback. As a proof of concept, a PV potential map for Cambridge, Massachusetts, USA, consisting of over 17,000 rooftops has been implemented as of September 2012. The new method constitutes the first linking of increasingly available geographic information system (GIS) and LiDAR urban datasets with the validated building performance simulation engine Daysim, thus-far used primarily at the scale of individual buildings or small urban neighbourhoods. A comparison of the new method with its predecessors reveals significant benefits as it produces hourly point irradiation data, supports better geometric accuracy, considers reflections from nearby urban context and uses predicted rooftop temperatures to calculate hourly PV efficiency. A validation study of measured and simulated electricity yields from two rooftop PV installations in Cambridge shows that the new method is able to predict annual electricity gains within 3.6–5.3% of measured production when calibrating for actual weather

data and detailed PV panel geometry. This predicted annual error using the new method is shown to be less than the variance which can be expected from climactic variation between years. Furthermore, because the new method generates hourly data, it can be applied to peak load mitigation studies at the urban level. This study also compares predicted monthly energy yields using the new method to those of preceding methods for the two validated test installations and on an annual basis for 10 buildings selected randomly from the Cambridge dataset.

14/01970 A review of voltage dip mitigation techniques with distributed generation in electricity networks

Ipinnimo, O. *et al. Electric Power Systems Research*, 2013, 103, 28–36.
The advent of power-quality sensitive equipment has made the provision of good power quality a real challenge across the globe. With the increasing use of sophisticated sensitive electronic equipment in industrial, residential and commercial sectors, it is important to protect them from any power-quality disturbance in order to avoid equipment damage and malfunction leading to financial loss for the customer. Voltage-quality disturbances, such as voltage dips, pose a serious concern as a power-quality problem, since due to their stochastic nature they cannot readily be eliminated from regular utility systems. However, they can be mitigated. High degree of penetration of distributed generation in power networks is useful in delivering different benefits to the utility in the form of ancillary services one of which is voltage dip mitigation in case of system contingencies. This paper presents a comprehensive review and comparison of various distributed generation schemes used by utilities for mitigation of voltage dips in power networks.

14/01971 Analysis of a novel gravity driven organic Rankine cycle for small-scale cogeneration applications

Li, J. *et al. Applied Energy*, 2013, 108, 34–44.
A naturally controlled organic Rankine cycle (ORC) without negative work is proposed. Compared with conventional ORCs, the novel system uses gravity instead of a pump to pressurize the working fluid, and hence the problems associated with the pump can be avoided. A possible application of the gravity driven ORC for combined heat and power generation is presented to outline the feasibility. Mathematical models are built. The required height for pressurization and the cycle efficiency varying with the condensation and evaporation temperatures are analysed on using R123, R245ca, R113, PF5050 and PF5060. The results reveal that on the same condition of operating temperature, the required height for pressurization may vary drastically when the working fluid is different. Fluid of high liquid density and low saturation pressure offers a low height. The power efficiency of the novel ORC is adequate for low temperature applications. With an expander efficiency of 75%, evaporation temperature of 100 °C and condensation temperature of 40 °C, the highest efficiency is about 10.2% with fluid of R123, which is 0.9% higher than that of the pump driven ORC. And the lowest required height is only about 20.9 m with fluid of PF5060. The proposed ORC has both cost and efficiency advantages.

14/01972 Chemical and structural stability of porous thin film NiO nanowire based electrodes for supercapacitors

Paravannoor, A. *et al. Chemical Engineering Journal*, 2013, 220, 360–366.
Nanowires of NiO were successfully synthesized using a simple hydrothermal route. The nanowires were characterized for phase composition and morphology by X-ray diffraction (XRD) and transmission electron microscopy (TEM) techniques, respectively. XRD analysis showed that the powders produced were of high purity cubic NiO phase. Selected area electron diffraction analysis during TEM showed the growth direction of NiO nanowires in (1 0 0), while exhibiting an average diameter of ~65 nm. Brunauer–Emmett–Teller analysis showed these nanowires exhibiting a surface area of 153.2 m^2/g. These nanowires were electrophoretically deposited on titanium foils as thin layer (~5 μm thickness) and were studied for their capacitive behaviour as electrodes for supercapacitor applications. Image analysis and atomic force microscopy studies revealed the thin-film coating to be highly porous (>50%). Cyclic voltammetry studies on these electrodes exhibited a specific mass capacitance of 750 F/g with 12% capacitance fade at the end of 1000 cycles. The present study elucidates how NiO surface morphology and OH^- adsorption/desorption behaviours underlying these electrodes impact the chemical and structural stability performance.

14/01973 Distribution network expansion considering distributed generation and storage units using modified PSO algorithm

Sedghi, M. *et al. International Journal of Electrical Power & Energy Systems*, 2013, 52, 221–230.
Multistage distribution network expansion because of load growth is a complex problem in distribution planning. The problem includes minimizing cost of objective function subject to technical constraints. The objective function consists of investment, operation and reliability costs. In this paper, HV/MV substations, main and reserve MV feeders, dispatchable distributed generation sources and storage units are considered as possible solutions for multistage distribution expansion planning. A three-load level is used for variable load and some strategies are proposed for distributed generation and storage units operation. A modified particle swarm optimization (PSO) algorithm is applied to solve the complex optimization problem. Numerical results of the case studies show the ability of the modification. Moreover, the proposed strategies improve the distribution network from both economical and reliability points of view compared with the other methods.

14/01974 Fuzzy sliding-mode based control (FSMC) approach of hybrid micro-grid in power distribution systems

Mohammadi, M. and Nafar, M. *International Journal of Electrical Power & Energy Systems*, 2013, 51, 232–242.
This paper presents modelling and control of a hybrid distributed energy sources including photovoltaic (PV), fuel cell (FC) and battery energy storage (BES) in a microgrid which provides both real and reactive power to support a utility grid. The overall configuration of the microgrid including dynamic models for the PV, FC, BES and its power electronic interfacing are briefly described. Then controller design methodologies for the power conditioning units to control the power flow from the hybrid power plant to the utility grid are presented. In order to distribute the power between power sources, the power sharing controller has been developed. The fuzzy sliding-mode control approach is proposed such that it can be applied with advantages to both fuzzy and sliding-mode controller. Simulation results are presented to demonstrate the effectiveness of the control strategy.

14/01975 Grid vulnerability analysis based on scale-free graphs versus power flow models

Correa, G. J. and Yusta, J. M. *Electric Power Systems Research*, 2013, 101, 71–79.
Graph theory techniques have emerged as useful tools in analysis of the physical performance of power grids, especially cascade failure events. Based on such models, several approaches have been proposed to estimate transmission network vulnerability. The most accepted methodologies rely on random error and deliberate attack tolerance assessment, conducted upon complex network paradigms. However, a lack of validation studies have been conducted for verification of the effectiveness of the results obtained with such methodologies, when applied to electric infrastructures. This paper investigates structural vulnerability by means of comparisons between physical power flow models and scale-free graph statistic indexes, generating conclusions on the appropriateness of graph theory techniques for assessment of electric network vulnerability. This is performed through simulations on standard IEEE bus-testing networks. A discussion of the utilization of several indexes in scale-free graphs for vulnerability assessment is also included.

14/01976 Heat load patterns in district heating substations

Gadd, H. and Werner, S. *Applied Energy*, 2013, 108, 176–183.
Future smart energy grids will require more information exchange between interfaces in the energy system. One interface where dearth of information exists is in district heating substations, being the interfaces between the distribution network and the customer building heating systems. Previously, manual meter readings were collected once or a few times a year. Today, automatic meter readings are available resulting in low cost hourly meter reading data. In a district heating system, errors and deviations in customer substations propagates through the network to the heat supply plants. In order to reduce future customer and heat supplier costs, a demand appears for smart functions identifying errors and deviations in the substations. Hereby, also a research demand appears for defining normal and abnormal heat load patterns in customer substations. The main purpose with this article is to perform an introductory analysis of several high resolution measurements in order to provide valuable information about substations for creating future applications in smart heat grids. One year of hourly heat meter readings from 141 substations in two district heating networks were analysed. The connected customer buildings were classified into five different customer categories and four typical heat load patterns were identified. Two descriptive parameters, annual relative daily variation and annual relative seasonal variation, were defined from each 1 year sequence for identifying normal and abnormal heat load patterns. The three major conclusions are associated both with the method used and the objects analysed. First, normal heat load patterns vary with applied control strategy, season, and customer category. Second, it is possible to identify obvious outliers compared to

normal heat loads with the two descriptive parameters used in this initial analysis. Third, the developed method can probably be enhanced by redefining the customer categories by their indoor activities.

14/01977 Influence of the voltage taps position on the self-field DC and AC transport characterization of HTS superconducting tapes

Vojenčiak, M. *et al. Cryogenics*, 2013, 57, 189–194.

The current–voltage (I–V) curve is the basic characteristic of a superconducting wire or tape. Measuring I–V curves is generally problematic when samples have poor stabilization. Soldering voltage taps to an active part of the conductor affects the effectiveness of the local cooling and/or can be difficult to do in certain devices such as fault current limiters and cables where the tapes are closely packed. In order to overcome these problems, voltage taps can be placed outside the active area of the superconductor. It was proved both by simulations and experiments that this arrangement leads to the same results as the standard four point method and it provides more detailed information for sample protection. The same arrangement can also be used for AC transport loss measurement. However in this case particular care has to be taken because the eddy current loss in the current leads contributes to the total measured loss. Numerical simulations were used to evaluate the contribution of the eddy current loss to the measured AC loss. With the help of simulations, one can determine whether the contribution of the eddy current loss is significant and possibly optimize the current leads to reduce that loss contribution.

14/01978 Integration of low-temperature transcritical CO_2 Rankine cycle in natural gas-fired combined cycle (NGCC) with post-combustion CO_2 capture

Ystad, P. A. M. *et al. International Journal of Greenhouse Gas Control*, 2013, 12, 213–219.

When integrating a natural gas-fired combined cycle with post-combustion CO_2 capture, an efficiency penalty is induced. In the current work the penalty was a reduction of net plant efficiency from 58.5% to 50.6%. The largest part of this penalty is related to the reduction of power output from the power plant due to steam consumption for CO_2 capture solvent regeneration. The potential of recovering low-temperature unused thermal energy is limited as this low-grade energy is at a temperature below the low-pressure pinch-point of the steam boiler. In this work, heat sources located in the CO_2 capture process and CO_2 compression process have been identified and integrated with a low-temperature Rankine cycle utilizing CO_2 as working fluid. The approach presented in this paper is novel in the sense that it has not been applied on power plants operating with post-combustion CO_2 capture. Results show that integration of the low-temperature CO_2 Rankine cycle can increase the net plant efficiency of a natural gas-fired combined cycle power plant by 1.6%-points (50.6–52.2%) when using a conventional monoethanolamine-based CO_2 capture process. Capture process modifications (lean vapour recompression) in combination with application of the CO_2 Rankine cycle can increase the efficiency by 1.8%-points (50.6–52.4%). The contribution from the CO_2 Rankine cycle for the latter case is 0.9%-points.

14/01979 Probabilistic model of polymer exchange fuel cell power plants for hydrogen, thermal and electrical energy management

Niknam, T. *et al. Journal of Power Sources*, 2013, 229, 285–298.

This paper proposes a probabilistic approach for economic/emission management of micro grids. In order to meet the electrical and thermal loads while having lower emission production in a more economical manner, combining heating and power along with hydrogen production and utilization strategies are employed. A proton exchange membrane fuel cell power plant (PEMFCPP) is considered as the prime mover of the combined heat and power system. The surplus power of PEMFCPP is managed to produce hydrogen. An electrochemical model for representation and performance evaluation of the proton exchange membrane fuel cell (PEMFC) is applied. Using this model, the output voltage and power of the PEMFC are calculated as a function of current, constructive and operational parameters. The proposed probabilistic optimization method includes $2m + 1$ point estimate method to cover the uncertainties and a modified multi-objective algorithm based on the modified gravitational search algorithm to find Pareto-optimal front of the operation management problem. The study considers the uncertainties in forecasted values of: the hourly market tariffs, electrical and thermal load demands, available output power of the photovoltaic and wind turbines units, fuel prices, hydrogen selling price, operation temperature of the fuel cell, and pressure of the reactant gases of fuel cells.

14/01980 Stress–strain behavior under static loading in Gd123 high-temperature superconductors at 77 K

Fujimoto, H. *et al. Cryogenics*, 2013, 57, 6–11.

Mechanical properties of melt-growth $GdBa_2Cu_3O_x$ (Gd123) superconducting samples with 10 wt% Ag_2O and 0.5 wt% Pt were evaluated at 77 K through flexural tests for specimens cut from the samples in order to estimate the mechanical properties of the Gd123 material without metal substrates, buffer layers or stabilization layers. The authors discuss the mechanical properties; the Young's modulus and flexural strength with stress–strain behaviour at 77 K. The results show that the flexural strength and fracture strain of Gd123 at 77 K are approximately 100 MPa and 0.1%, respectively, and that the origin of the fracture is defects such as pores, impurities and non-superconducting compounds. The authors also show that the Young's modulus of Gd123 is estimated to be 160–165 GPa.

14/01981 Structural and electrochemical properties of single crystalline MoV_2O_8 nanowires for energy storage devices

Shahid, M. *et al. Journal of Power Sources*, 2013, 230, 277–281.

This study reports the synthesis of MoV_2O_8 nanowires of high quality using spin coating followed by the thermal annealing process. Transmission electron microscopy (TEM) reveals the average diameter of synthesized nanowire about 100 nm, and average length ranges from 1 to 5 μm. The TEM analysis further confirms the ⟨001⟩ growth direction of MoV_2O_8 nanowires. The electrochemical properties of synthesized nanowires using cyclic voltammetry show the specific capacitance 56 Fg^{-1} at the scan rate of 5 $mV\,s^{-1}$ that remains 24 Fg^{-1} at 100 $mV\,s^{-1}$. The electrochemical measurements suggest that the MoV_2O_8 nanowires can be used as a material for the future electrochemical capacitors (energy storage devices).

14/01982 The role of dialogue in fostering acceptance of transmission lines: the case of a France–Spain interconnection project

Ciupuliga, A. R. and Cuppen, E. *Energy Policy*, 2013, 60, 224–233.

It is a recognized fact that the lack of public and political support is one of the main sources of delay in building new transmission lines. In an energy era where there is an increasing lag between transmission grid development and the rapid generation growth, it is essential to streamline the related transmission line approval procedures. There is a strong relationship between stakeholder engagement on one side, and acceptance and support on the other side. The aim of the paper is to investigate ways of fostering acceptance of transmission lines through participation by analysing in detail the case of a disputed France–Spain interconnection project. The authors argue that participatory processes should embrace not only an instrumental rationale, but also normative and substantive rationales. Based on literature and the case study, this authors analyse this important condition for effective participation in transmission planning procedures.

14/01983 Thermal gasification or direct combustion? Comparison of advanced cogeneration systems in the sugarcane industry

Deshmukh, R. *et al. Biomass and Bioenergy*, 2013, 55, 163–174.

This study compares different cogeneration system scenarios for efficient energy production from bagasse fuel in an Indonesian sugar and ethanol factory. These scenarios include the use of condensing-extraction steam turbines, variable speed electric drives for process equipment, measures to reduce low pressure steam demand for process needs, and two advanced cogeneration systems. One advanced system includes an 80 bar high pressure direct combustion steam Rankine cycle (advanced SRC), while the other uses a biomass integrated gasifier combined cycle (BIGCC); both utilize fuel dryers. Using steady-state thermodynamic models, it is estimated that the net electricity generation potentials of the BIGCC and advanced SRC systems are approximately seven and five times the potential of the existing factory, respectively. The maximum net electricity generation potentials for the respective systems are 170 kWh/tc (BIGCC) and 140 kWh/tc (advanced SRC). However, the BIGCC system needs a bagasse feed rate that is 50% higher than the advanced SRC system to satisfy the factory low-pressure steam demand for sugar and ethanol processing, which may affect its ability to provide steam and electricity during the off-season. For the Indonesian sugar factory, the annual revenue potential of the BIGCC system is US$14 million per year, approximately 50% higher than that of the advanced SRC system (electricity sale rate: US$45/MsWh; carbon credit price: US$13.60). BIGCC technology is still in an early stage of development and there are no commercial systems in sugar factories, so an advanced SRC system may be a more suitable option in the near future.

14/01984 Use of FRP pultruded members for electricity transmission towers

Godat, A. *et al. Composite Structures*, 2013, 105, 408–421.

This study investigates the replacement of traditional materials (steel, wood and concrete) in electricity transmission lines by fibre-glass pultruded members. The first part of the study summarizes a comparison between different design approaches to experimental data

for glass-fibre pultruded sections. For this purpose, a total of 15 specimens made of E-glass and either polyester or vinylester matrix are tested: (i) angle-, square- and rectangular-section specimens are subjected to axial compression and (ii) I- and W-section specimens are tested under bending. The experimental results are summarized in terms of the failure mode, critical buckling load and load–displacement relationships. Design equations available in fibre-reinforced polymer (FRP) design manuals and analytical methods proposed in the literature are used to predict the critical buckling load and compared to the experimental results. Design of various FRP pultruded sections and cost estimate are conducted for 69 kV electricity transmission portal frame and a total distance of 10 km. The significance of the present findings with regard to economic solutions is discussed.

Economics, policy, supplies, forecasts

14/01985 A highly resolved modeling technique to simulate residential power demand

Muratori, M. *et al. Applied Energy*, 2013, 107, 465–473.

This paper presents a model to simulate the electricity demand of a single household consisting of multiple individuals. The total consumption is divided into four main categories, namely cold appliances, heating, ventilation, and air conditioning, lighting, and energy consumed by household members' activities. The first three components are modelled using engineering physically based models, while the activity patterns of individuals are modelled using a heterogeneous Markov chain. Using data collected by the US Bureau of Labor Statistics, a case study for an average US household is developed. The data are used to conduct an in-sample validation of the modelled activities and a rigorous statistical validation of the predicted electricity demand against metered data is provided. The results show highly realistic patterns that capture annual and diurnal variations, load fluctuations, and diversity between household configuration, location, and size.

14/01986 A model for long-term electricity expansion planning with endogenous environmental costs

Santos, H. L. and Legey, L. F. L. *International Journal of Electrical Power & Energy Systems*, 2013, 51, 98–105.

This paper describes a methodology to incorporate the environmental costs associated to the construction and operation of power plants in the long-term expansion planning process of hydrothermal generation systems. These external costs are estimated in terms of monetary values, according to the nature of their impacts and endogenously included in the formulation of the expansion planning model. The minimization of the maximum regret framework used in the modelling process enables the development of a single expansion strategy that allows for corrections in the expansion trajectory, according to the behaviour of electricity demand. A case study based on the Brazilian system and previous environmental valuation studies is presented and discussed. The results found contemplate a reduction in the total cost of the electricity system expansion planning.

14/01987 A reexamination of renewable electricity policy in Sweden

Fridolfsson, S.-O. and Tangerås, T. P. *Energy Policy*, 2013, 58, 57–63.

Green certificates are the main instrument for promoting renewable electricity (RES-E) in Sweden. But certificates cover only a limited share of total RES-E production. Under partial coverage, crowding out may arise whereby costly new RES-E replaces inexpensive old RES-E. Granting certificates to all of RES-E production improves efficiency, but leaves windfall rent to otherwise profitable facilities. The transaction costs in the permit process for new RES-E in Sweden are also analysed. Municipalities veto socially desirable projects because of asymmetrically distributed investment costs and benefits. The authors propose market-based permit fees rather than limited veto rights as a solution to this 'not-in-my-backyard' problem.

14/01988 Economic merits of a state-of-the-art concentrating solar power forecasting system for participation in the Spanish electricity market

Kraas, B. *et al. Solar Energy*, 2013, 93, 244–255.

Forecasts of power production are necessary for the electricity market participation of concentrating solar power (CSP) plants. Deviations from the production schedule may lead to penalty charges. Therefore, the accuracy of direct normal irradiance (DNI) forecasts is an important issue. This paper elaborates the mitigation impact on deviation penalties of an electricity production forecasting tool for the 50 MW_{el} parabolic trough plant Andasol 3 in Spain. Only few commercial DNI forecast schemes are available nowadays. One of them, based on a model output statistics (MOS) forecast for the period July 2007 to December 2009, is assessed and compared to the zero cost 2-day persistence approach, which assumes yesterday's weather conditions and electricity generation also for the following day. The quality of the meteorological forecasts is analysed both with forecast verification methods and from the perspective of a power plant operator. Using MOS, penalties in the study period are reduced by 47.6% compared to the 2-day persistence case. Finally, typical error patterns of existing MOS forecasts and their financial impact are discussed. Overall, the paper aims at quantifying the economic value of nowadays readily available numerical weather prediction in this use case. A special feature of the study is its focus on a real market case and the use of real data, rather than following a purely academic approach, and thus to provide some new insights regarding the economic benefit of using and improving state-of-the-art forecasting techniques.

14/01989 Forecasting electricity infeed for distribution system networks: an analysis of the Dutch case

Tanrisever, F. *et al. Energy*, 2013, 58, 247–257.

Estimating and managing electricity distribution losses are the core business competencies of distribution system operators (DSOs). Since electricity demand is a major driver of network losses, it is essential for DSOs to have an accurate estimate of the electricity in-feed in their network. In this paper, motivated by the operations of a Dutch electricity distribution system operator, the authors examine how to estimate the electricity in-feed in distribution networks one year in advance with hourly forecasting intervals, so that the DSOs may effectively hedge for their physical losses in the wholesale markets. They identify the relevant factors for DSOs to forecast the electricity in-feed in their networks, and to quantify their effects. The authors show that most of the calendar variables, such as national holidays, long weekends as well as days near holidays have a significant effect on electricity in-feed. This analysis reveals that the impact of calendar variables significantly depends on the hour of the day. On the other hand, economic and demographic factors do not seem to influence the electricity in-feed for the planning horizon of DSOs. The authors also explore the influence of meteorological factors on the electricity in-feed in the Netherlands. Finally, they develop and compare methods for electricity in-feed forecasting, based on multiple regression and time series analysis. This analysis reveals that the regression-based method outperforms the time series-based method on the average measures whereas the time series-based method is better in the worst case analysis. Hence, the forecasting methods used by DSOs may have significant implications on their financial hedging policies.

14/01990 Forecasting electricity price volatility with the Markov-switching GARCH model: evidence from the Nordic electric power market

Cifter, A. *Electric Power Systems Research*, 2013, 102, 61–67.

In this paper, electricity price behaviour in the Nordic electric power market is forecasted with both the Markov-switching generalized autoregressive conditional heteroskedasticity (MS-GARCH) model and a set of different volatility models. The MS-GARCH model is estimated with two regimes, representing periods of low and high volatility. This study shows that electricity price volatility is not only highly volatile but also strongly regime-dependent. The empirical results show that the MS-GARCH model enables more accurate forecasting than the standard GARCH models, according to tail loss and reality check tests for one- and multi-step ahead forecasts. The results suggest that both the electricity generation companies and consumers of electricity could carry out better price forecasts by using the proposed MS-GARCH model.

14/01991 Fulfilling the electricity demand of electric vehicles in the long term future: an evaluation of centralized and decentralized power supply systems

Brouwer, A. S. *et al. Applied Energy*, 2013, 107, 33–51.

Electric vehicles (EVs) are currently seen as an option for a more sustainable transportation sector, but it is not yet clear how to supply them with electricity whilst striving for low costs and low CO_2 emissions. Renewable sources can supply electricity with low emissions, but their penetration rate is still insufficient to meet current demand, let alone the extra demand of EVs. A promising option is supply by combined heat and power (CHP) plants with high combined efficiencies, but an in-depth evaluation of the benefits of combining of EVs and CHP plants is still missing. Therefore, this study evaluates the performance of four different types of CHP plants to power electric vehicles, as compared to use of electricity from the grid. The performance of CHP plants is simulated using detailed datasets of the composition of a future power system, the demand for household electricity and heat, and technical specifications of CHP plants and electric vehicles. The lowest abatement costs of 60–190 €/tCO_2 were found to be achieved with grid electricity based on a low-carbon electricity mix compared to a business-as-usual electricity mix with marginal emissions of 450–500 gCO_2/kW h. When electricity is supplied

by CHP plants, emissions are −1000 to 400 gCO_2/kW h, and abatement costs are 165–940 €/tCO_2. Added benefits of joint implementation of CHP plants and EVs were not observed in this study: the timing of CHP electricity supply and EV electricity demand did not match well, and abatement costs were not lowered.

14/01992 Least cost 100% renewable electricity scenarios in the Australian national electricity market

Elliston, B. *et al. Energy Policy*, 2013, 59, 270–282.

Least-cost options are presented for supplying the Australian national electricity market (NEM) with 100% renewable electricity using wind, photovoltaics, concentrating solar thermal (CST) with storage, hydroelectricity and biofuel-powered gas turbines. The authors use a genetic algorithm and an existing simulation tool to identify the lowest cost (investment and operating) scenarios of renewable technologies and locations for NEM regional hourly demand and observed weather in 2010 using projected technology costs for 2030. These scenarios maintain the NEM reliability standard, limit hydroelectricity generation to available rainfall, and limit bioenergy consumption. The lowest cost scenarios are dominated by wind power, with smaller contributions from photovoltaics and dispatchable generation: CST, hydro and gas turbines. The annual cost of a simplified transmission network to balance supply and demand across NEM regions is a small proportion of the annual cost of the generating system. Annual costs are compared with a scenario where fossil fuelled power stations in the NEM today are replaced with modern fossil substitutes at projected 2030 costs, and a carbon price is paid on all emissions. At moderate carbon prices, which appear required to address climate change, 100% renewable electricity would be cheaper on an annual basis than the replacement scenario.

14/01993 Mixed integer non-linear programming and artificial neural network based approach to ancillary services dispatch in competitive electricity markets

Canizes, B. *et al. Applied Energy*, 2013, 108, 261–270.

Ancillary services represent a good business opportunity that must be considered by market players. This paper presents a new methodology for ancillary services market dispatch. The method considers the bids submitted to the market and includes a market clearing mechanism based on deterministic optimization. An artificial neural network is used for day-ahead prediction of regulation down, regulation up, spin reserve and non-spin reserve requirements. Two test cases based on California independent system operator data concerning dispatch of regulation down, regulation up, spin reserve and non-spin reserve services are included in this paper to illustrate the application of the proposed method: (1) dispatch considering simple bids and (2) dispatch considering complex bids.

14/01994 Modelling the impact of EVs on electricity generation, costs and CO_2 emissions: assessing the impact of different charging regimes and future generation profiles for Ireland in 2025

Calnan, P. *et al. Energy Policy*, 2013, 61, 230–237.

This paper focuses on the impact of electric vehicles (EVs) on electricity generation in Ireland in 2025 based on five alternative generation portfolios. The year 2025 was selected for assessment due to the information on the composition of the five generation portfolios from Eirgrid the system operator in Ireland being provided. Detailed market simulations were undertaken on the five possible generation portfolios to assess the impact of government targets for EVs on the generation costs, emissions, generation stack and the cost to load of this additional demand. This paper also studied the impact between a standard and least-cost EV loading regime to ascertain the benefits that could be achieved. The results show that gas will be the dominant source of electricity generation to load EVs and that wind as an electricity source will experience a minor reduction in curtailment, with the least-cost charging profile showing a more pronounced reduction. The capital benefits of the 'standard' and 'least-cost EV' load are found to be negligible. The portfolios studied generated CO_2 emissions per kilometre between 52 and 70 gCO_2/km. All portfolios with the exception of coal were found to comply with European Union regulation 443/2009.

14/01995 One size does not fit all: averaged data on household electricity is inadequate for residential energy policy and decisions

Carlson, D. R. *et al. Energy and Buildings*, 2013, 64, 132–144.

Residential electricity users need more detail than monthly bills to reduce consumption. With the emergence of technologies that provide detailed usage estimates for energy consumption, two questions arise. First, how many different energy-consuming appliances contribute to household electricity load, and secondly which appliances? Using national average penetration rates, the Residential Energy Consumption Survey (RECS), estimates that 42 unique appliances account for 93% of electricity consumption, while 12 appliances account for 80% of average household electric load. A typical scenario is developed from national and regional penetration rates and find that eight appliances are responsible for 80% of a household's electric load in the USA. Four household scenarios are developed: a house that uses electric appliances, gas appliances, the average household, and typical household. It is concluded that RECS cannot be used as a representative household as it overestimates the number of appliances that contribute to a household electric load. The number of significant appliances is affected by appliance ownership and use, which is more variable between homes than between census divisions. These results can be used to design and maximize the value of residential energy information and management systems.

14/01996 Potentials and challenges in implementing feed-in tariff policy in Indonesia and the Philippines

Bakhtyar, B. *et al. Energy Policy*, 2013, 60, 418–423.

Located in Southeast Asia, Indonesia and the Philippines are characterized by a tropical climate and high amounts of rainfall that render their high potential for hydro-power and wind energy deployment. The volcanic geography of both countries also indicates their high geothermal potential compared with that of other countries, and their high solar radiation level makes them suitable areas to establish power plants. The present study is an archival-statistical overview of the potential generation of renewable energy in Indonesia and the Philippines and the implementation of the feed-in tariff (FiT) policy. This research focuses on the challenges encountered by politicians and policymakers and confirms the insufficient production of energy from wind, solar, and bio-gas sources despite the potential and the attempts to deploy FiT. Results show that the role of the government in providing support to investors is not clear in both countries. In addition, inflation rates have not been calculated. However, FiT has benefitted both countries by preventing degression during the primary years.

14/01997 Residential winter kW h responsiveness under optional time-varying pricing in British Columbia

Woo, C. K. *et al. Applied Energy*, 2013, 108, 288–297.

A large sample of daily electricity consumption and pricing data are available from a pilot study conducted by BC Hydro in British Columbia, Canada, of its residential customers under optional time-varying pricing and remotely activated load-control devices for the four winter months of November 2007 to February 2008. This study uses the data to estimate the elasticity of substitution σ, defined as the negative of the percentage change in the peak-to-off-peak kW h ratio due to a 1% change in the peak-to-off-peak price ratio. These estimates of σ characterize residential price responsiveness with and without load control during cold-weather months. While the estimates of σ without load control are highly statistically significant ($\alpha = 0.01$), they are less than 0.07. With load control in place, however, these σ estimates more than triple. Finally, the authors show that time-varying pricing without load control causes a peak kW h reduction of 2.6% at the 2 : 1 peak-to-off-peak price ratio to 9.2% at the 12 : 1 peak-to-off-peak price ratio. Load control raises these reduction estimates to 9.2% and 30.7%.

14/01998 SuperGrid or SmartGrid: competing strategies for large-scale integration of intermittent renewables?

Blarke, M. B. and Jenkins, B. M. *Energy Policy*, 2013, 58, 381–390.

This paper defines and compares two strategies for integrating intermittent renewables: SuperGrid and SmartGrid. While conventional energy policy suggests that these strategies may be implemented alongside each other, the paper identifies significant technological and socio-economic conflicts of interest between the two. The article identifies differences between a domestic strategy for the integration of intermittent renewables, *vis-à-vis* the SmartGrid, and a cross-system strategy, *vis-à-vis* the SuperGrid. Policy makers and transmission system operators must understand the need for both strategies to evolve in parallel, but in different territories, or with strategic integration, avoiding for one strategy to undermine the feasibility of the other. A strategic zoning strategy is introduced from which attentive societies as well as the global community stand to benefit. The analysis includes a paradigmatic case study from west Denmark which supports the hypothesis that these strategies are mutually exclusive. The case study shows that increasing cross-system transmission capacity jeopardizes the feasibility of SmartGrid technology investments. A political effort is required for establishing dedicated SmartGrid innovation zones, while also redefining infrastructure to avoid the narrow focus on grids and cables. SmartGrid investment trusts could be supported from reallocation of planned transmission grid investments to provide for the equitable development of SmartGrid strategies.

14/01999 The impact of electricity storage on wholesale electricity prices

Nyamdash, B. and Denny, E. *Energy Policy*, 2013, 58, 6–16.

This paper analyses the impact of electricity storage on the production cost of a power system and the marginal cost of electricity (electricity price) using a unit commitment model. Also, real-world data have been analysed to verify the effect of storage operation on the electricity price using econometric techniques. The unit commitment model found that the deployment of a storage system reduces the fuel cost of the power system but increases the average electricity price through its effect on the power system operation. However, the reduction in the production cost was found to be less than the increase in the consumer's cost of electricity resulting in a net increase in costs due to storage. Different storage and CO_2 price scenarios were investigated to study the sensitivity of these results. The regression analysis supports the unit commitment results and finds that the presence of storage increases average wholesale electricity prices for the case study system.

14/02000 Transmission planning by minimizing curtailment of market transactions
Gunnaasankaraan, H. *et al. Electric Power Systems Research*, 2013, 101, 1–8.
Congestion in the transmission network prevents execution of the desired market transactions. This results in some of the market transactions having to be curtailed, which translates into a loss to customers. This paper suggests that the decision to expand transmission facilities will depend on the loss sustained by the customer due to curtailment of market transactions vs cost of installing new transmission facilities over a planning period. Thus, in a power system, the sum total cost of investment to expand transmission facilities and cost of cumulative loss due to curtailment of transactions to all the customers is set up as a minimization problem, which results in optimal transmission expansion needed over a planning period. With this consideration, the Benders decomposition technique is used for transmission expansion planning by taking investment cost as the master problem and loss due to curtailment of market transactions as the slave problem. The southern Brazil power system is used as a test case where this methodology has been employed.

07 STEAM RAISING

Boiler operation/design

14/02001 A comparison between exergetic and economic criteria for optimizing the heat recovery steam generators of gas-steam power plants
Carapellucci, R. and Giordano, L. *Energy*, 2013, 58, 458–472.
Combined-cycle gas turbines (CCGT) are gaining an increasingly important role in power generation thanks to their high thermal efficiency, low installed cost and ready availability. Increasing natural gas prices, the optimization of CCGT operating parameters is becoming a topic of growing interest. In this paper two different methodologies for optimizing CCGTs are compared. The first aims to minimize the cost per unit of electricity generated, the second to minimize an objective function based on exergoeconomic principles accounting for the costs related with thermodynamic inefficiencies. Optimization results have been obtained considering different CCGT configurations, with single or multi-pressure heat recovery steam generators (HRSG), and varying the gas turbine technology, fuel price and plant capacity factor. A modular approach has been adopted to design a highly effective and flexible HRSG layout, in terms of number of pressure levels and arrangement of heat exchange sections along the flue gas path, together with the corresponding energy, exergy and cost balances, using an 'interaction matrix', with nodes between elementary components and towards the surrounding environment.

14/02002 A droplet model in steam condensation with noncondensable gas
Lan, Z. *et al. International Journal of Thermal Sciences*, 2013, 68, 1–7.
A physical and revised mathematical droplet model with respect to molecular clustering is proposed to describe the state of steam molecules before condensing on the cooled solid surface in steam condensation in the presence of non-condensable gas (NCG). Based on the Dillmann and Meier homogeneous nucleation model, introducing the wall conditions and making some correlations, the mathematical model was used to calculate the size distribution of clusters and describe the effect of the presence of NCG on the distribution of clusters. The heat transfer model considering the effect of interfacial effects was used to calculate the shape and temperature of clusters. The predicted results of Gibbs free energy at different subcooling degrees and different saturated temperatures were given. The model explains the effect of NCG on condensation heat transfer performance and the predicted results are in agreement with the experimental results reported in the literature. That confirms the validity of the model.

14/02003 Alternative venting in steam retorts – an approach to energy savings in thermal processing
Berteli, M. N. *et al. Chemical Engineering and Processing: Process Intensification*, 2013, 70, 204–210.
The venting operation in retorts operating under steam pressure is an important step in the sterilization process and it aims to steam flush the air from inside the equipment in order to ensure sterilization safety. This part of the process is short in time but intensive in steam consumption, and hence this study evaluated an alternative venting operation based on the use of water to displace the air, aimed at reducing this energy consumption. The objective was to evaluate the energy consumption in a steam retort loaded with thermally convective and conductive products, comparing the conventional and alternative venting processes. The steam flow rates showed that the alternative venting process reduced steam consumption by up to 50% as compared to conventional venting.

14/02004 Hydrothermal carbonization of sewage sludge for energy production with coal
Parshetti, G. K. *et al. Fuel*, 2013, 111, 201–210.
Hydrothermal carbonization using subcritical water (250 °C, 8–10 MPa and 15 min reaction time) was investigated to recover solid carbonaceous fuel, i.e. sludge char (HT-SL) from urban sewage sludge. The carbonaceous HT-SL had an energy–density of 15.82 MJ kg^{-1}. For achieving maximum waste-to-energy conversion, the co-combustion of HT-SL with low-rank Indonesian coal (LRIC) and hydrothermally upgraded LRIC (HT-LRIC) was investigated using a thermogravimetric analyser (TGA) and the emission characteristics of gaseous pollutants were determined by using coupled Fourier transform infrared spectroscopy (FTIR). To gain insights into the physicochemical and microstructure properties, carbonaceous fuel were characterized by proximate, ultimate, field emission scanning electron microscopy, FTIR, X-ray diffraction, Brunauer–Emmett–Teller and inductively coupled plasma optical emission spectrometry analysis. Conventional TGA and kinetic parameters such as activation energy of various LRIC, HT-LRIC and HT-SL blends were also determined. This fundamental study provides a basic insight into co-combustion of HT-SL with LRIC and HT-LRIC, which forms a scientific basis for the efficient utilization of sewage sludge as an energy source while minimizing greenhouse gas emissions.

14/02005 Inner tube optimization of double-tube once-through steam generator
Wei, X. *et al. International Journal of Heat and Mass Transfer*, 2013, 59, 93–102.
The study presenting in this paper considers a double-tube once-through steam generator with an outer straight tube and an inner helical tube. For the purpose of the compact structure and lower pressure drop, the inner helical tube is optimized. The tube length and the combined pressure drop are considered as the two objective functions, and the pitch of the inner helical tube is considered as a design parameter. The multi-objective optimization model is established and translated into a single-objective function by the objective product method. The single-objective function is optimized by fmincon routine in Matlab software. The optimal pitches of the helical tube vary in sub-cooled region, boiling region and superheated region. The results show that the smaller pitch brings shorter tube length and higher pressure drop, and the effects are strong in sub-cooled region and superheated region, but weak in the boiling region.

14/02006 Internal flow and heat transfer of a condensing water droplet in steam flow
Yang, Z. *et al. Chemical Engineering Science*, 2013, 94, 54–59.
The growth of a condensing water droplet of millimetre-size in steam flow is experimentally measured using a charge-coupled device camera. The growth rate of the droplet is found to increase with the steam flowrate, which disagrees with previous theories. A computational fluid dynamics model is developed to simulate the internal flow and heat transfer of the droplet, and it predicts the droplet growth rate increases with the steam flowrate in good agreement (about 2% in deviation) with the experimental results. It is demonstrated that the steam shearing at the droplet surface causes an internal flow in the droplet. The internal flow, though small (less than 1% of the external steam flow in magnitude), convects the temperature profiles to the droplet bottom and causes a 10–25% enhancement in the heat transfer of the droplet. For droplets of the same bottom, the steam shearing effect is more significant with a larger droplet height.

14/02007 Mass transfer coefficients considering effects of steam in oxy-fuel combustion of coal char
Yu, J. *et al. Fuel*, 2013, 111, 48–56.
Considering the effects of Stefan flow and steam in the oxy-fuel combustion of char, correction factors for the mass transfer coefficients of gas reactants, O_2, CO_2 and H_2O, are derived in the present work. By comparisons with the experimental data, the rigid continuous-film model, and the uncorrected single-film model, it is concluded that the corrections greatly improve the predictions of the particle temperature, combustion rates and burnout time. The correction factors are related to the gas components, reaction numbers and rate ratios. Generally, the increase of number and rate of surface reaction will result in the enhancement of Stefan flow and hence decrease the mass transfer coefficients. But discussion under the typical conditions of oxy-fuel combustion shows that different reaction has different impacts on the mass transfer of reactive gases. In the presence of steam, the correction for O_2 is nearly the same as cases neglecting the steam, owing to the low gasification rate of H_2O and the accelerative diffusion transfer of O_2 in H_2O and H_2. The correction for CO_2 increases slightly by about 3% because the gasification rate of H_2O is only a little higher than that of CO_2. On the contrary, the participation of O_2 and CO_2 reactions plays considerable role in the mass transfer coefficient of H_2O. Especially, the high rate reaction, like O_2 oxidation, has more remarkable effects on the mass transfer of gas reactants. Therefore, more attention should be paid to the modification of mass transfer coefficients when the O_2 oxidation reaction is prevailing in the char oxy-fuel combustion, for the transfer coefficients will be greatly changed.

14/02008 Optimization of thermoelectric topping combined steam turbine cycles for energy economy
Yazawa, K. *et al. Applied Energy*, 2013, 109, 1–9.
A mismatch between the fuel combustion temperature ~2250 K (adiabatic) and the high-pressure steam temperature up to 900 K, results in a large amount of thermodynamic losses in steam turbine (ST) cycles. A solid-state thermoelectric (TE) placed on top of a ST cycle will produce additional electrical power. By selecting the right materials for the TE generator for high temperature operation, the energy production from the same fuel consumption will increase. Recent nano-structured enhancements to the thermoelectric materials could provide practical performance benefits. This study carried out a theoretical study on the optimization of the interface temperature connecting these two idealized engines for energy economy as a combined system. It also analytically studied the optimum point-of-operation between the maximum power output for minimizing the payback and the maximum efficiency to obtain the maximum fuel economy for each generator. The economic optimum ends up in a significant reduction in energy cost ($/kW h). The combined TE topping generator system provides a lower energy cost for any period of operational life and higher interface temperature compared to the ST cycle alone. The maximum power output is observed at around 700 K of interface temperature for 10,000 h of operation, while the minimum energy production cost from the combined system is observed at over 900 K with $ZT = 1$.

08 COMBUSTION

Burners, combustion systems

14/02009 A new pilot absorber for CO_2 capture from flue gases: measuring and modelling capture with MEA solution
Sønderby, T. L. *et al. International Journal of Greenhouse Gas Control*, 2013, 12, 181–192.
A pilot absorber column for CO_2 recovery from flue gases was constructed and tested with aqueous 30 wt% monoethanolamine (MEA), a primary amine, as capture solvent. The pilot plant data were compared with a mathematical rate based packed-column model. The simulation results compared well with the pilot plant data. The packed height of the column can be varied from 1.6 to 8.2 m by means of five different liquid inlets. The column has an inner diameter of 100 mm and is packed with structured Mellapak 250Y packing. Counter-current flow is used. The pilot plant performance was investigated by changing three parameters: the absorption height, liquid flow rate, and the loading of lean MEA. This was done using a synthetic flue gas consisting of 10% CO_2 with a flow rate of approximately 33 m^3/h at ambient temperature and atmospheric pressure. 23 runs were performed. It was observed that while CO_2 recovery increases with an increase in flow rate of absorbent and absorption height, it decreases as the lean CO_2-loading of the absorbent increases. In addition it has been possible to obtain temperature bulges in the bottom part of the absorber by the applied operation conditions. Bulges are observed at liquid flows around 4.2 L/min and below. The results showed that it was possible to achieve 80% recovery with 3.3 m absorption height and a liquid flow of 2.1 L/min. The simulations show good agreement with the experimental values, although slight deviations arise as the CO_2-loading increases and the temperature bulge becomes more distinct.

14/02010 A simulation study of coal combustion under O_2/CO_2 and O_2/RFG atmospheres in circulating fluidized bed
Zhou, W. *et al. Chemical Engineering Journal*, 2013, 223, 816–823.
The Euler–Euler modelling approach was employed to simulate the coal combustion in a circulating fluidized bed combustor. The unsteady processes of gas–solid two-phase flow, heat transfer, mass transfer and chemical reactions were considered. By numerical simulation, distributions of pressure, solid volume fraction, temperature and gas concentrations (O_2, CO_2, H_2O, CO, NO and SO_2) were studied in O_2/CO_2 combustion mode (mixture of O_2 and CO_2 from gas bottles as oxidant) and O_2/RFG combustion mode (mixture of O_2 and recycled flue gas as oxidant) with O_2 concentration range of 21–40%. Calculations were made for two cases, maintaining the same coal feed rate and maintaining the same oxidant volume flow rate. Simulated temperature distribution, pressure distribution and outlet gas concentrations were validated by the experimental data in 30% O_2/70% CO_2 atmosphere.

14/02011 An experimental study of combustion and emissions of biomass pellets in a prototype pellet furnace
Roy, M. M. *et al. Applied Energy*, 2013, 108, 298–307.
This study presents combustion and emission results obtained using a prototype pellet furnace with 7–32 kW capacity (designed for burning high ash content pellet fuels) for four biomass pellets: one grass pellet and three wood pellets. Fuel property, gas emissions and furnace efficiency are compared. In regard to fuel properties, proximate analysis, ultimate analysis and heating values are determined and emissions of carbon monoxide (CO), nitric oxide (NO), nitrogen dioxide (NO_2), nitrogen oxides (NO_x) and sulfur dioxide (SO_2) are measured and compared. Scanning electron microscopy was used for ash analysis. No ash agglomeration was observed and ash discharge was in the form of powder instead of lumped particles, which are usually observed for high ash biomass fuel. The results suggest that grass pellets can successfully be combusted with similar performance and emissions to that of other wood pellets if burned in appropriate combustion installations.

14/02012 Comparisons of different heat transfer models of a walking beam type reheat furnace
Singh, V. K. and Talukdar, P. *International Communications in Heat and Mass Transfer*, 2013, 47, 20–26.
Four different heat transfer models (models 1–4) for the prediction of temperature of the slabs of a walking beam type reheat furnace have been compared. The models are classified based on the solution methodology and simplifications. In the first three models (models 1–3), the furnace is modelled as radiating medium with spatially varying known temperature. Model 1 solves the three-dimensional transient conduction in the slab and radiation in the furnace separately and is coupled via the boundary condition. In the second model, both radiation in the furnace and conduction in the slab are solved simultaneously. A user-defined function programme has been developed to process the movement of the slabs. Model 3 is similar to model 2 but it includes additionally the skid support systems for the slabs. In model 4, convection in the furnace has been included in addition to all the features considered in model 3. The convection has been modelled with the consideration of flow of hot gas through the inlet of the burners. All the models have been compared for their performance and computational time. Model 1 has been found to be quite economical and accurate. The inclusion of a skid-supporting system has little effect in the temperature distribution in the slab.

14/02013 Configuration effects of natural gas fired multi-pair regenerative burners in a flameless oxidation furnace on efficiency and emissions
Cho, E.-S. *et al. Applied Energy*, 2013, 107, 25–32.
This study reports on the characteristics of heat transfer and emissions in natural gas fired flameless oxidation conditions created using multiple semi-industrial regenerative burners. Burner positions and firing modes (parallel and staggered) are varied, and their effects on efficiency, emissions (NO, CO) and temperature uniformity are studied. Also the excess air ratio and the cycle time have been varied. The operation uses two burner pairs together to provide 200 kW_{th} giving a volumetric heat release closely resembling real industrial operating conditions (48 MW/m^3). The parallel mode operation shows

better results concerning low emission of CO and NO, and uniform temperature distribution in the furnace. On the other hand, the staggered mode operation showed a comparatively low performance due to a developed unsymmetrical flow pattern in the furnace. Single digit NO emission was measured for the parallel mode with low CO concentration due to low and uniform temperature. CO concentration is strongly dependent on the burner cycle time because the switching of burners generates periods of unstable and non-uniform flow pattern and also temperature distribution temporarily. The numerical simulation with skeletal reaction showed typical reaction characteristics of flameless oxidation, which is a slow and uniform reaction progress in the furnace. Meanwhile, the reaction model needs to improve its accuracy because the reaction speed appears to be slower than the experiment, and the simulation of a case showed extinguished reaction. The comparable simulation results also showed an order higher CO emission and an order lower NO emission, which is assumed to be related with low reaction kinetics.

14/02014 CO_2 quality control in oxy-fuel combustion: a dynamic study on the absorption of SO_2 into sodium based aqueous solutions relevant to scrubbing prior to CO_2 compression

Liu, D. *et al. International Journal of Greenhouse Gas Control*, 2013, 12, 2–8.

Oxy-fuel combustion is an emerging technology to mitigate CO_2 emissions from power plants. Compared with other CO_2 capture technologies, gas impurities in oxy-fuel flue gas are highly concentrated, among which SO_2 is of concern. Dynamic transient experiments have been conducted in a semi-batch well stirred reactor (WSR) relevant to the conditions of the flue gas scrubbers operating at atmospheric pressure prior to CO_2 compression in oxy-fuel technology for carbon dioxide capture and storage. SO_2 in N_2 as well as in CO_2 were considered. The initial pH of the solutions considered was those of NaOH (with concentrations of 0.01 and 1 M), Na_2CO_3 (0.005 M) and $NaHCO_3$ (0.01 M). Analysis of the liquid solutions showed that the concentration of bicarbonate increases with pH at a pH greater than 5.5 indicating a loss of effectiveness of the sodium reagent. A practical discharge pH of the liquid discharge from the scrubber is also higher than 4 as at a lower pH the absorption rate of SO_2 reduced. This operating range is consistent with the reported operating range of the scrubber used in the Vattenfall oxy-fuel pilot plant.

14/02015 Effect of oxygen enrichment on acid gas combustion in hydrogen/air flames under Claus conditions

Selim, H. *et al. Applied Energy*, 2013, 109, 119–124.

Results are presented to examine the combustion of acid gas (H_2S and CO_2) in hydrogen-fuelled flames using a mixture of oxygen and nitrogen under Claus conditions ($\phi = 3$). Specifically the effect of oxygen enrichment in the above flames is examined. The compositions of acid gas examined are 100% H_2S and 50% H_2S/50% CO_2 with different percentages of oxygen enrichment (0%, 19.3% and 69.3%) in the oxygen/nitrogen mixtures. The results revealed that combustion of acid gas formed SO_2 wherein the mole fraction of SO_2 increased to an asymptotic value at all the oxygen concentrations examined. In addition, increase in oxygen enrichment of the air resulted in increased amounts of SO_2 rather than the formation of more desirable elemental sulfur. In case of 50% H_2S/50% CO_2 acid gas, carbon monoxide mole fraction increased with oxygen enrichment which is an indicator to the availability of additional amounts of oxygen into the reaction pool. This gas mixture resulted in the formation of other sulfurous–carbonaceous compounds (COS and CS_2) due to the presence of carbon monoxide. The results showed that the rate of COS formation increased with oxygen enrichment due to the availability of higher amounts of CO while that of CS_2 reduced. The global reactions responsible for this observed phenomenon are presented.

14/02016 Energy analysis and environmental impacts of a MSW oxy-fuel incineration power plant in China

Tang, Y. T. *et al. Energy Policy*, 2013, 60, 132–141.

The entire life cycle of a municipal solid waste (MSW) oxy-fuel incineration power plant was evaluated using the method of life cycle assessment (LCA) to identify and quantify the fossil energy requirements and environmental impacts. The functional unit was 1000 kg MSW. During the life cycle, the saving standard coal by electricity generation was more than diesel consumption, and the effect of soot and ashes was the greatest among all calculated categorization impacts. The total weighted resource consumption and total weighted environment potential of MSW oxy-fuel incineration were −0.37 mPR_{90} (milliperson equivalent) and −0.27 PET_{2010} (person equivalent), better than MSW incineration with CO_2 capture via monoethanolamine absorption. The sensitivity analysis showed that the electric power consumption of air separation unit (ASU) was the primary influencing parameter, and the influence of electric power consumption of CO_2 compressor was secondary, while transport distance had small influence. Overall, MSW oxy-fuel incineration technology has certain development potential with the increment of MSW power supply efficiency and development of ASU in the future.

14/02017 Group additivity in soot formation for the example of C-5 oxygenated hydrocarbon fuels

Barrientos, E. J. *et al. Combustion and Flame*, 2013, 160, (8), 1484–1498.

Sooting tendencies have been measured for 29 compounds with five carbon atoms and different oxygen contents, along with 12 additional oxygenated pure compounds and 10 blends of commercial fuels. The test compounds include alcohols, ethers, aldehydes, ketones, acids, esters, keto-esters and hydroxy-esters. The threshold sooting index (TSI), as defined and used in the literature, was primarily used to quantify the sooting tendency of the compounds. It is shown that this index does not account for the presence of oxygen atoms in the fuel molecules, and the impact of fuel oxygen on the stoichiometric air requirement. The application of the TSI to oxygenated fuels leads to sooting tendencies inconsistent with those reported in the literature. A new sooting index is proposed for oxygenated and non-oxygenated compounds, which considers the relation between the height of the flame tip and the volumetric stoichiometric air requirement of the flame. This new index is called the oxygen extended sooting index (OESI). The results obtained by this new index corroborate that not only the oxygen content but also the molecular structure has an influence on the sooting tendency of fuels. Different functional groups, not only those including oxygen atoms, impart different sooting tendencies. A structural group contribution approach based on group additivity is proposed to interpret experimental observations on the effect of oxygen functional groups on the sooting tendency of fuels using the example of C-5 oxygenated fuels. Groups with a higher fraction of carbon–carbon bonds showed a higher contribution to the sooting tendency than those with a higher concentration of carbon–hydrogen bonds. Among the C-5 mono-oxygenated compounds, the sooting tendency increased in this order: aldehydes < alcohols < ketones < ethers < *n*-alkanes and for the C-5 di-oxygenated compounds, the sooting tendency order was: acids < esters < di-ethers. In general, both unsaturated and branched compounds showed slight increases in sooting tendency with respect to their saturated and linear counterparts. Finally, the new sooting index was applied to commercial biofuel blends (denatured ethanol–gasoline and soybean-derived biodiesel–diesel) and empirical correlations were obtained.

14/02018 Mixing and segregation of binary oxygen carrier mixtures in a cold flow model of a chemical looping combustor

Alghamdi, Y. A. *et al. Chemical Engineering Journal*, 2013, 223, 772–784.

In a typical chemical looping combustion process, the oxygen for fuel combustion is supplied by circulating metal based oxygen carriers between two interconnected fluidized bed reactors. The redox characteristics of oxygen carriers and hence the overall performance of the process can be significantly improved by utilizing binary mixtures of oxygen carrier particles. The full potential of such multi-species particle systems however can be only realized when particles segregation is minimized. This study is concerned with gaining an understanding of the mixing and segregation behaviour of binary mixtures of oxygen carrier particles with different sizes and densities in a cold flow model representing a 10 kWth chemical looping combustor. The hydrodynamics of such systems were investigated and compared with a typical chemical looping combustion process where single species are used. This was followed by investigating the solids mixing and segregation behaviour in terms of segregation intensity and species weight percentage at each reactor as a function of operating parameters. It was shown that increasing the total solid inventory, particle terminal velocity ratio, composition, and air reactor superficial velocity increases the riser pressure, solid circulation rates, and riser solid holdup. Mixing and segregation regimes of the fuel reactor and the component segregation between the two reactors were also mapped. The results showed that, for mixtures of species with low terminal velocity to high terminal velocity ratios of greater than 0.7, a good mixing in the fuel reactor can be achieved by maintaining the superficial gas velocity to the mixture minimum fluidization velocity ratio above 5. For the tested conditions, the component segregation between the two reactors was avoided by maintaining the ratio of the riser superficial velocity to the terminal velocity of the species with a high terminal velocity between 1.25 and 2.

14/02019 Mixtures of rubber tyre and plastic wastes pyrolysis: a kinetic study

Miranda, M. *et al. Energy*, 2013, 58, 270–282.

This study aimed at analysing the possible routes for pyrolysis reaction mechanisms of polymeric materials, namely rubber tyres and plastic wastes (polyethylene, polypropylene and polystyrene). Consequently, seeking sustainable transformation of waste streams into valuable

chemicals and renewable liquid fuels, a mixture of 30% rubber tyre, 20% polyethylene, 30% polypropylene and 20% polystyrene was subjected to pyrolysis. Different kinetic models were studied using experimental data. None of the mechanisms found in the literature led to a numerical adjustment and different pathways were investigated. Kinetic studies were performed aimed at evaluating the direct conversions into new solid, liquid and gaseous products and if parallel reactions and/or reversible elementary steps should be included. Experiments were performed in a batch system at different temperatures and reaction times. Kinetic models were evaluated and reaction pathways were proposed. The models reasonably fit the experimental data and explain waste thermal degradation. Kinetic parameters were estimated for all temperatures and dependence of E_a and pre-exponential factor on temperature was evaluated. The rate constant of some reactions exhibited non-linear temperature dependence on the logarithmic form of Arrhenius law. This fact strongly suggests that temperature has a significant effect on reaction mechanism of pyrolysis of mixtures of rubber tyre and plastic wastes.

14/02020 Multi-scale modeling of Claus thermal furnace and waste heat boiler using detailed kinetics

Manenti, F. *et al. Computers & Chemical Engineering*, 2013, 59, 219–225.

The modelling of thermal reaction furnaces of sulfur recovery units (SRUs) is a rather complex problem since it involves different modelling scales such as the kinetic/molecular scale, the reactor scale, and the chemical process scale. This work introduces the multi-scale modelling approach to characterize the kinetic and reaction engineering scales for the thermal section of SRUs, involving the reactor furnace and the waste heat boiler. Specifically, also the waste heat boiler is modelled using detailed kinetics to characterize the recombination effects, which cannot be neglected any longer since they significantly influence the outlet compositions. The proposed models are validated on experimental and literature data for the kinetic scale. The reactor scale is validated on the industrial data coming from SRUs operating in Nanjing and Mumbai plants.

14/02021 Nitrogen and sulphur chemistry in pressurised flue gas systems: a comparison of modelling and experiments

Normann, F. *et al. International Journal of Greenhouse Gas Control*, 2013, 12, 26–34.

Nitrogen and sulfur chemistry is more significant during the compression of flue gases than when they are under atmospheric conditions. This fact became apparent during the development of oxy-fuel power plant technology to capture carbon dioxide (CO_2). In the oxy-fuel power plant, the CO_2-rich flue gas stream is compressed to enable efficient transport and storage. During this process, NO_x and SO_x are removed as acids in the condensed water. However, the chemistry of these steps is not understood well enough to allow for control and design of the process. In this study, the gas- and liquid-phase chemistry of NO_x and SO_x at elevated pressures were evaluated by comparing a state-of-the-art reaction mechanism to the results of experimental investigations. The model used confirms previous observations of substantial absorption of NO_x and SO_x and subsequent formation of acids in pressurized flue gas systems. The results of the modelling show that the oxidation of NO into NO_2 governs the absorption of NO_x. The complex chemistry of the liquid phase, which includes reactions between HNO_2, H_2SO_3, and possibly H_2SO_4, is critical for the rate of absorption of NO_x and SO_x from the gas to the liquid phase. This process is heavily dependent on the pH level. The modelling suggests that N_2O is formed as a stable product through the liquid-phase reactions.

14/02022 Novel perspectives on the dynamics of premixed flames

Blumenthal, R. S. *et al. Combustion and Flame*, 2013, 160, (7), 1215–1224.

The present study develops an alternative perspective on the response of premixed flames to flow perturbations. In particular, the linear response of laminar premixed flames to velocity perturbations is examined in the time domain, and the corresponding impulse response functions are determined analytically. Different flame types and shapes as well as different velocity perturbation models are considered. Two contributions to the flame response are identified: a convective displacement of the flame due to velocity perturbations, and a restoration mechanism, which is a consequence of the combined effects of flame propagation and flame anchoring. The impulse responses are used to identify the relevant time scales and to form non-dimensional frequencies. The link of the present results to previous studies formulated in the frequency domain is established. The time domain approach is found to facilitate analysis and interpretation of well-known properties of premixed flames such as excess gain, periodic cutoff and self-similar aspects of flame response. Characteristic time scales of response appear naturally and can be interpreted in a straightforward manner.

14/02023 Partitioning of selected trace elements in coal combustion products from two coal-burning power plants in the United States

Swanson, S. M. *et al. International Journal of Coal Geology*, 2013, 113, 116–126.

Samples of feed coal (FC), bottom ash (BA), economizer fly ash (EFA), and fly ash (FA) were collected from power plants in the Central Appalachian basin and Colorado plateau to determine the partitioning of As, Cr, Hg, Pb, and Se in coal combustion products (CCPs). The Appalachian plant burns a high-sulfur (about 3.9 wt%) bituminous coal from the Upper Pennsylvanian Pittsburgh coal bed and operates with electrostatic precipitators (ESPs), with flue gas temperatures of about 163 °C in the ESPs. At this plant, As, Pb, Hg, and Se have the greatest median concentrations in FA samples, compared to BA and EFA. A mass balance (not including the FGD process) suggests that the following percentages of trace elements are captured in FA: As (48%), Cr (58%), Pb (54%), Se (20%) and Hg (2%). The relatively high temperatures of the flue gas in the ESPs and low amounts of unburned C in FA (0.5% loss-on-ignition for FA) may have led to the low amount of Hg captured in FA. The Colorado plateau plant burns a blend of three low-S (about 0.74 wt%) bituminous coals from the Upper Cretaceous Fruitland Formation and operates with fabric filters (FFs). Flue gas temperatures in the baghouses are about 104 °C. The elements As, Cr, Pb, Hg and Se have the greatest median concentrations in the fine-grained fly ash product (FAP) produced by cyclone separators, compared to the other CCPs at this plant. The median concentration of Hg in FA (0.0983 ppm) at the Colorado plateau plant is significantly higher than that for the Appalachian plant (0.0315 ppm); this higher concentration is related to the efficiency of FFs in Hg capture, the relatively low temperatures of flue gas in the baghouses (particularly in downstream compartments), and the amount of unburned C in FA (0.29% loss-on-ignition for FA).

14/02024 Performance of CLOU process in the combustion of different types of coal with CO_2 capture

Adánez-Rubio, I. *et al. International Journal of Greenhouse Gas Control*, 2013, 12, 430–440.

Chemical-looping with oxygen uncoupling (CLOU) process is a chemical-looping combustion (CLC) technology that allows the combustion of solid fuels using oxygen carriers with inherent CO_2 separation. The oxygen necessary for the fuel combustion is supplied by a solid oxygen carrier, which contains a metal oxide. The oxygen carrier circulates between two interconnected fluidized reactors: the fuel and the air reactor. In the CLOU process, the oxygen carrier releases gaseous oxygen in the fuel reactor which burns coal as in common combustion with air, so the CO_2 generated is undiluted with N_2. The reduced oxygen carrier is oxidized by air to the initial metal oxide in the air reactor, then being ready to start a new cycle. The aim of this work is to study the performance of the CLOU process using coals of different rank. Experiments were carried out in a continuously operated 1.5 kW_{th} unit. Particles prepared by spray drying containing 60 wt% CuO were used as oxygen carrier. Four coals of different rank (anthracite, low volatile bituminous, medium volatile bituminous and lignite) were used as fuel. Besides, the temperature in the fuel reactor was varied between 900 and 950 °C. In all the experiments there was complete combustion of the coal to CO_2 and H_2O, without any unburnt product. The carbon capture efficiency greatly depends on the coal rank and fuel reactor temperature. High carbon capture efficiencies were obtained for lignite and medium volatile bituminous coals. The maximum capture efficiency was 99.3% at 950 °C with lignite. The analysis of the experimental results was used to evaluate the effect of the coal rank in a CLOU system when a carbon separation system is included. At 925 °C, the solid inventory needed to reach 95% of CO_2 capture efficiency with a carbon separation system of 90% of efficiency is 45 kg/MW_{th} using lignite, 85 kg/MW_{th} using MV bituminous, 140 kg/MW_{th} using LV bituminous and 490 kg/MW_{th} using anthracite. It must be pointed out the low solid inventories needed in the CLOU process for the different coal rank analysed in this work.

14/02025 Photocatalytic degradation of soot deposition: self-cleaning effect on titanium dioxide coated cementitious materials

Smits, M. *et al. Chemical Engineering Journal*, 2013, 222, 411–418.

Diesel soot emissions deteriorate the appearance of architectural building materials by soot fouling. This soot deposition devalue the aesthetic value of the building. A solution to counteract this problem is applying titanium dioxide on building materials. TiO_2 can provide air-purifying and self-cleaning properties due to its photocatalytic activity. In literature, photocatalytic soot oxidation is observed on glass or silicon substrates. However, degradation of soot by photocatalysis was not yet investigated on cementitious samples (mortar, concrete)

although it is one of the most frequently used building materials. In this study, photocatalytic soot oxidation by means of TiO_2 coated cementitious samples is addressed. The soot removal capacity of four types of TiO_2 layers, coated on mortar samples, is evaluated by means of two detection methods. The first method is based on colorimetric measurements, while the second method uses digital image processing to calculate the area of soot coverage. The experimental data revealed that cementitious materials coated with commercially available TiO_2 exhibited self-cleaning properties as it was found that all coated samples were able to remove soot. The P25 coating gave the best soot degradation performance, while the Eoxolit product showed the slowest soot degradation rate. In addition, gas chromatography measurements in a closed chamber experiment with P25 confirmed that complete mineralization of about 60% of the soot was obtained within 24 h since CO_2 was the sole observed oxidation product. Due to its realistic approach, this study proves that photocatalytic soot removal on TiO_2 coated cementitious surfaces is possible in practice, which is an important step towards the practical application of self-cleaning building materials.

14/02026 Predictions of CO and NO_x emissions from steam cracking furnaces using GRI2.11 detailed reaction mechanism – a CFD investigation

Hassan, G. *et al. Computers & Chemical Engineering*, 2013, 58, 68–83.
This investigation develops a three-dimensional computational fluid dynamics (CFD) model to simulate the turbulent diffusion flame on the fire-side of the radiation section of a thermal cracking test furnace coupled with a non-premixed low NO_x floor burner. When this type of burners which uses the internal flue gas recirculation (FGR) technique is coupled with large scale furnaces, both the turbulent mixing and chemical reaction rates are comparable and hence this should be considered in the model. Different combustion models are used to simulate the turbulence–chemistry interactions for this flame. The CFD model, based on the eddy dissipation concept (EDC) combustion model coupled with the detailed GRI2.11 reaction mechanism, gives the most reasonable predictions compared with the available experimental data or empirical correlations for the diffusion flame in the thermal cracking test furnace, especially for the flame length and the CO and NO_x emissions.

14/02027 Pyrolysis kinetics and reactivity of algae–coal blends

Kirtania, K. and Bhattacharya, S. *Biomass and Bioenergy*, 2013, 55, 291–298.
This paper presents results from a thermogravimetric analysis and modelling based study using a fresh water alga, *Chlorococcum humicola*, and a victorian brown coal and their blends at different proportions. Pyrolysis was studied using the pure coal and pure algae as well as their blends to a final temperature of 1000 °C at different heating rates to understand the kinetics. The kinetic data of pure algae and pure coal were used to predict the pyrolysis characteristics of coal–algae blends at various heating rates using a modified distributed activation energy model which closely matched the experimental data. The experimental results also indicate that there is no chemical interaction between the algae and coal during pyrolysis.

14/02028 Scalar transport in diffusion flame wrapped up by an air and fuel side vortex

Mishra, S. *et al. International Communications in Heat and Mass Transfer*, 2013, 47, 32–40.
The present work involves a computational study of soot (chosen as a scalar which is a primary pollutant source) formation and transport in a laminar acetylene diffusion flame perturbed by a convecting line vortex. The topology of soot contours resulting from flame vortex interactions has been investigated. More soot was produced when vortex was introduced from the air side in comparison to the fuel side. Also, the soot topography was spatially more diffuse in the case of the air-side vortex. The computational model was found to be in good agreement with the experimental work previously reported in the literature. The computational simulation enabled a study of various parameters such as temperature, equivalence ratio and temperature gradient affecting the soot production and transport. Temperatures were found to be higher in the case of the air-side vortex in contrast to the fuel-side one. In the case of the fuel-side vortex, abundance of fuel in the vortex core resulted in fuel-rich combustion zone in the core and a more discrete soot topography. The overall soot production also was observed to be low in the fuel-side vortex. However, for the air-side vortex, air abundance in the core resulted in higher temperatures and greater soot production. Probability density functions have been introduced to investigate the spatiotemporal variation of soot yield and transport and their dependence on temperature and acetylene concentration from statistical point of view. In addition, the effect of flame curvature on soot production is also studied. The regions convex to fuel stream-side demonstrated a thicker soot layer.

14/02029 Solution of radiative inverse boundary design problem in a combined radiating-free convecting furnace

Mosavati, B. *et al. International Communications in Heat and Mass Transfer*, 2013, 45, 130–136.
In this paper, an inverse boundary design problem of combined natural convection–radiation is solved. The aim of this paper is to find the strength of heaters in a step-like enclosure to produce desired temperature and heat flux distribution on the design surface. The finite volume method for transition flow (which causes a faster convergence) is used as the direct solver of the energy and momentum equations. The SIMPLE algorithm is utilized to satisfy pressure–velocity coupling in order to solve the free convection heat transfer. Also, the backward Monte Carlo method is employed in order to be able to compute the distribution factors and carry out the radiant exchange calculations. Finally, the goal function, which is defined on the basis of square root error, is minimized by means of conjugate gradients method. The effects of variation of range of parameters such as the Rayleigh number, temperature ratio, radiation conduction parameter and the emissivity coefficient of insulated surfaces on the relative root mean square and heat flux are investigated and results are compared. The results demonstrate the efficiency and the accuracy of the proposed method.

14/02030 Soot temperature and *KL* factor for biodiesel and diesel spray combustion in a constant volume combustion chamber

Zhang, J. *et al. Applied Energy*, 2013, 107, 52–65.
This paper presents measurements of the soot temperature and *KL* factor for biodiesel and diesel combustion in a constant volume chamber using a two-colour technique. This technique uses a high-speed camera coupled with two narrowband filters (550 and 650 nm, 10 nm FWHM). After calibration, statistical analysis shows that the uncertainty of the two-colour temperature is less than 5%, while it is about 50% for the *KL* factor. This technique is then applied to the spray combustion of biodiesel and diesel fuels under an ambient oxygen concentration of 21% and ambient temperatures of 800, 1000 and 1200 K. The heat release result shows higher energy utilization efficiency for biodiesel compared to diesel under all conditions; meanwhile, diesel shows a higher pressure increase due to its higher heating value. Biodiesel yields a lower temperature inside the flame area, a longer soot lift-off length, and a smaller soot area compared to diesel. Both the *KL* factor and the total soot with biodiesel are lower than with diesel throughout the entire combustion process, and this difference becomes larger as the ambient temperature decreases. Biodiesel shows approximately 50–100 K lower temperatures than diesel at the quasi-steady stage for 1000 and 1200 K ambient temperature, while diesel shows a lower temperature than biodiesel at 800 K ambient. This result may raise the question of how important the flame temperature is in explaining the higher NO_x emissions often observed during biodiesel combustion. Other factors may also play an important role in controlling NO_x emissions. Both biodiesel and diesel temperature measurements show a monotonic dependence on the ambient temperature. However, the ambient temperature appears to have a more significant effect on the soot formation and oxidation in diesel combustion, while biodiesel combustion soot characteristics shows relative insensitivity to the ambient temperature.

14/02031 The influence of high intensity solar radiation on the temperature and reduction of an oxygen carrier particle in hybrid chemical looping combustion

Jafarian, M. *et al. Chemical Engineering Science*, 2013, 95, 331–342.
The temperature variations during the conversion of an oxygen carrier particle exposed to high intensity solar heat flux are assessed as a function of time with an unsteady-state model. The conservation equations of energy and mass are solved simultaneously using an appropriate numerical technique, whose reliability was assessed by comparison with the available experimental and numerical data from the literature. This model was used to study the effect on the particle conversion and maximum temperature of various operating parameters, i.e. particle size, external heat and mass transfer, radiation heat flux intensity, CH_4 mole fraction and surrounding temperature. The numerical results show that exposing the particle to high flux solar radiation decreases the conversion time and increases the particle temperature. The calculations indicate that a higher Nusselt number results in a lower temperature rise of the particle and a lower conversion time. The calculations also show that, convection is the dominant mechanism of particle cooling, despite the high temperature of the particle surface.

14/02032 Thermal model for the optimization of a solar rotary kiln to be used as high temperature thermochemical reactor

Tescari, S. *et al. Solar Energy*, 2013, 95, 279–289.

The present study focuses on a thermal model describing a rotary kiln reactor. Several applications can be foreseen for this reactor, for example high temperature heat storage for thermal solar power plants. The energy is provided by concentrated solar radiation that heats up the cavity walls. A thermal model, describing the reactor behaviour, is developed and validated. Particular attention is given to the radiation model, which constitutes the most important heat transfer. An innovative way of modelling the reactor aperture through a fictive surface at an imposed equivalent temperature leads to a significant decrease of the simulation time, without decreasing the precision of the solution. The model is validated by comparison first with other models, which make different assumptions and second with experimental results. After the validation, the model can be used for simulating the behaviour under different operating condition or to define the possible improvements by a change of the reactor geometry such as the insulation's thermal conductivity or thickness.

14/02033 Wettability study in CO_2 capture from flue gas using nano porous membrane contactors

Hassanlouei, R. N. *et al. International Journal of Greenhouse Gas Control*, 2013, 16, 233–240.

Wettability of nanoporous membrane contactors that are exposed to different chemical solvents was studied in this research. The work is conducted using computational simulation of CO_2 capture from flue gas in a hollow-fibre membrane module. the computational fluid dynamics method was applied for numerical solution of governing transport equations. Simulations were performed to study CO_2 transport through membrane for complete wetting and non-wetting conditions. Simulation results were validated through comparing with the experimental data for CO_2 capture using amine aqueous solutions. The simulation results were inconsistent with the experimental data. To investigate the influence of solvent on separation performance, six common chemical absorbents including aqueous solutions of diethanolamine, N-methyldiethanolamine, monoethanolamine, 2-amino-2-methyl-1-propanol, sodium hydroxide and potassium glycinate were considered in the simulation. The simulation results revealed that the capture of CO_2 using aqueous solution of potassium glycinate was the highest among the absorbents.

Fire safety

14/02034 Curvature and confinement effects for flame speed measurements in laminar spherical and cylindrical flames

Bonhomme, A. *et al. Combustion and Flame*, 2013, 160, (7), 1208–1214.

This paper discusses methods used to obtain laminar flame speeds in spherical laminar premixed flames. Most recent studies express the laminar flame consumption speed as $\rho_b/\rho_u dR/dt$, where R is the flame radius and ρ_b/ρ_u is the ratio of the burnt to the fresh gas density (ρ_b is evaluated at chemical equilibrium and supposed to be constant). This paper investigates the validity of this assumption by reconsidering it in a more general framework. Other formulae are derived and tested on a direct numerical simulation of cylindrical flames (methane/air and octane/air). Results show that curvature and confinement effects lead to variations of ρ_b and ρ_u and to significant errors on the flame speed. Another expression (first proposed by Bradley and Mitcheson in 1976) is derived where no density evaluation is required and only pressure and flame radius evolution are used. It is shown to provide more precise results for the consumption speed than $\rho_b/\rho_u \mathrm{d}R/\mathrm{d}t$ because it takes into account curvature and confinement of the flame in the closed bomb.

14/02035 Direct estimation of diffuse gaseous emissions from coal fires: current methods and future directions

Engle, M. A. *et al. International Journal of Coal Geology*, 2013, 112, 164–172.

Coal fires occur in nature spontaneously, contribute to increases in greenhouse gases, and emit atmospheric toxicants. Increasing interest in quantifying coal-fire emissions has resulted in the adaptation and development of specialized approaches and adoption of numerical modelling techniques. Overview of these methods for direct estimation of diffuse gas emissions from coal fires is presented in this paper. Here the stochastic Gaussian simulation was used to interpolate CO_2 fluxes measured using a dynamic closed chamber at the Ruth Mullins coal fire in Perry County, Kentucky, USA. This approach allows for preparing a map of diffuse gas emissions, one of the two primary ways that gases emanate from coal fires, and establishing the reliability of the study both locally and for the entire fire. Future research directions include continuous and automated sampling to improve quantification of gaseous coal-fire emissions.

14/02036 Evaluation of simple models of flame radiation in the frame of fire propagation

Collin, A. and Boulet, P. *International Journal of Heat and Mass Transfer*, 2013, 59, 83–92.

Simple models for radiative transfer evaluation in the frame of flame propagation are discussed and evaluated through comparisons with a complete absorbing–emitting volume flame model. The cases of the solid flame model and of the optically thin flame are considered as they are usually involved in fire propagation studies. It is shown that the solid flame model provides satisfactory results in some applications, but only for flames with sufficiently high optical thickness (above three at least). However, its inability to model the intensity distribution when shifting from the normal to the flame surface and its inaccuracy when addressing the case of low or even moderate optical thicknesses are two weaknesses that should be kept in mind when using this model. Regarding the optically thin flame model, it is demonstrated that its use should be restricted to really low optical thicknesses, far below one, which makes the application of such models quite unrealistic unless for small-scale flames. The true absorbing–emitting flame treatment should be preferred, with moderate supplementary cost regarding computational integration, if combined with dedicated methods like a reciprocal Monte Carlo method as presented here for example.

14/02037 Flame length elongation behavior of medium hydrocarbon pool fires in cross air flow

Hu, L. *et al. Fuel*, 2013, 111, 613–620.

This paper presents an experimental investigation on flame lengths of medium pool fires under horizontal cross air flows. Square pool fires with dimensions of 10, 15, 20 and 25 cm, using ethanol and heptane as typical fuels, are burned under cross air flows ranged in 0–2.5 m/s. The burning rates are measured by an electronic balance with accuracy of 0.1 g. The flame geometrical characteristics are recorded by a charge-coupled device digital camera, in which the mean flame length is quantified based on flame appearance intermittency spatial distribution. Results show that the cross air flow enhances the mass burning rate in a linear function of flow speed. Such enhancement effect is more prominent, indicated by a higher enhancement rate (β), for heptane than that for ethanol. This fuel type effect on β can be accounted for by a thermochemical property heat release parameter of the fuel (R, ratio of heat of combustion to heat of effect evaporation, $R = \Delta H_c/\Delta H_{fg}$). The normalized value of β/R is in a linear function of reciprocal of pool length ($\beta/R \sim d^{-1}$) and independent of fuel. The flame length is found to be elongated by the cross air flow due to the enhancement of the fuel burning (evaporation), as also being more remarkable for heptane than ethanol. A generalized model is proposed to approximate the elongated flame length (ℓ_f), in relation to an amended dimensionless Froude number incorporating globally both the thermochemical property, molecular property and reaction molar stoichiometric ratio of the fuel, as well as the ambient oxygen molar concentration factor.

14/02038 Modeling fire-induced radiative heat transfer in smoke-filled structural cavities

Jiang, Y. *et al. International Journal of Thermal Sciences*, 2013, 66, 24–33.

Accurate heat transfer prediction is important to structural fire engineering in order to analyse thermal–mechanical behaviour of structures in fire. However, the presence of cavities and participating media complicates radiative calculations. A numerical approach with finite element and discrete ordinates method is presented in this paper to predict fire imposed radiative heat fluxes to these type of structural members. This approach is used to simulate heat transfer to unprotected steel I-sections with symmetrical cavities exposed to post-flashover fires. Results show that the cavity geometry could strongly attenuate the radiative energy, while the presence of hot smoke enhances radiative transfer by emission. Average radiative fluxes for inner surfaces of the I-sections are seen to increase with smoke opacity. In addition, the radiative fluxes are observed to decrease faster for I-sections with higher section factors. This work also shows that the self-radiating mechanism of I-sections is important in the optically thin region, and existing methodologies neglecting these physics could significantly underestimate steel temperatures.

14/02039 The effect of polymeric binder on composite propellant flame structure investigated with 5 kHz OH PLIF

Hedman, T. D. *et al. Combustion and Flame*, 2013, 160, (8), 1531–1540.

High-speed (5 kHz) planar laser-induced fluorescence (PLIF) and high-resolution imaging are used to probe the flame structure and to image coarse ammonium perchlorate (AP) particles on the surface of deflagrating bimodal composite propellants formulated with various binders. Three binder systems are examined: hydroxyl-terminated polybutadiene (HTPB), polybutadiene acrylonitrile (PBAN) and dicyclopentadiene (DCPD). A comparison of coarse AP particle behaviour and flame structure is presented for each propellant over a pressure range of 1–6.4 atm. Individual AP particle ignition delay, burn

time and flame heights are quantified. Both jet-like diffusion flames and lifted, over-ventilated flames were observed for the propellants examined. The average diffusion flame height is observed to increase gradually over the pressure range studied. differential scanning calorimetry and thermogravimetric analysis was also performed on the AP/binder systems. It was found that both AP/HTPB and AP/PBAN react together exothermically while AP/DPCD reacts independently, with a quick binder pyrolysis proceeding AP decomposition. Propellants formulated with HTPB, PBAN and DCPD were found to possess a similar diffusion flame structure, but those with DCPD were measured to have a significantly higher burning rate. Propellants formulated with DCPD were observed to routinely eject coarse AP crystals from the burning surface, which results in the higher burning rate. Based on experimental observations, it is argued that either fast binder pyrolysis or poor adhesion to coarse AP particles is the mechanism responsible for the particle ejection.

09 PROCESS HEATING, POWER AND INCINERATION

Energy applications in industry

14/02040 An ontological approach towards enabling processing technologies participation in industrial symbiosis

Raafat, T. *et al. Computers & Chemical Engineering*, 2013, 59, 33–46.
A new ontological framework which supports processing technologies participation in industrial symbiosis (IS) is proposed. The framework uses semantic web service formalism to describe technology based on tacit knowledge embedded in the domain ontology and explicit knowledge acquired from the users. To enhance technology discovery, IS relevant processing technology classification and characterization is proposed. Technology participation in IS is addressed. Partial semantic input–output matching is used to propose complex and innovative networks assessed and ranked by their technological, economic and environmental benefits. The proposed framework is implemented as a web service and operation demonstrated using a case study.

14/02041 Analysis of the characteristics of the residues of the wine production chain finalized to their industrial and energy recovery

Toscano, G. *et al. Biomass and Bioenergy*, 2013, 55, 260–267.
In Italy it is estimated that 1.5 Tg of dry matter residues are produced by the agri-food sector. Approximately 30% of them are represented by residues of wine industry sector: grape marc. Referring to its production, it is possible to evaluate about 10 Mg of grapes from each vineyard hectare that generate, as wine industry residue, 2.7 Mg of grape marc, corresponding to about 19 GJ in terms of energy content. This kind of biomass is heterogeneous and composed of stalks, grape skins and seeds. In this paper, in order to investigate the possibility of an energy and industrial utilization, the physical-chemical characteristics of each single component of grape marc are examined. In addition, a mechanical extraction test on the seed was performed to evaluate the vegetable oil production and the characteristics of the cake. Results on grape marc components put in evidence some difference in terms of ash and chemical elements content, which represent, specifically for these materials, the most critical aspects to take into account in combustion heating systems.

14/02042 CFD simulations of dense solid–liquid suspensions in baffled stirred tanks: prediction of solid particle distribution

Tamburini, A. *et al. Chemical Engineering Journal*, 2013, 223, 875–890.
Industrial tanks devoted to the mixing of solid particles into liquids are often operated at an impeller speed N less than N_{js} (defined as the lowest speed allowing the suspension of all particles): under such conditions the distribution of solid-particles is very far from being homogeneous and very significant concentration gradients exist. The present work is devoted to assessing the capability of computational fluid dynamics (CFD) in predicting the particle distribution throughout the tank. A CFD model proposed elsewhere and successfully applied to the prediction of the sediment amount and shape was adopted here to simulate the particle distribution under partial-to-complete suspension conditions. Both transient (via the sliding grid approach) and steady-state (via the multiple reference frame approach) RANS simulations were carried out for the case of a flat-bottomed baffled tank stirred by a Rushton turbine. Results show that the model can reliably predict the experimental particle distribution at all investigated impeller speeds. Transient simulations were found to predict slightly better the experimental data with respect to steady state simulations. Radial gradients of solids concentration, usually neglected in the literature, where found to be significant in the presence of unsuspended solid particles settled on the vessel bottom (i.e. incomplete suspension conditions).

14/02043 Characteristics of integrated micro packed bed reactor-heat exchanger configurations in the direct synthesis of dimethyl ether

Hayer, F. *et al. Chemical Engineering and Processing: Process Intensification*, 2013, 70, 77–85.
The performance of three integrated micro-packed bed reactor-heat exchangers (IMPBRHEs) for direct DME synthesis over physical mixtures of CuO–ZnO–Al_2O_3 and γ-Al_2O_3 catalysts was experimentally investigated. Systematic variations in reactor and slit dimensions and configuration were analysed in terms of thermal behaviour, mass transfer, pressure drop and residence time distribution (RTD). The pressure drop was always small (<0.12 bar) relative to the total pressure (50 bar), and linear dependence with GHSV confirms the predicted laminar flow for $Re = 0.1$–2. A narrow RTD was estimated by the dispersion analysis. Careful temperature measurements confirmed that the reaction temperature is mainly controlled by the oil heat exchange to give a practically uniform temperature profile for set inlet oil temperatures of 220–320 °C. The micro-packed beds were found free of the internal as well as external mass transfer limitations, as showed by no significant change in the CO conversion and dimethyl ether (DME) yield for different catalyst particle sizes, no effect of varying the linear gas velocity, and no effect of manipulating reactant diffusion coefficient. Packed bed microstructured reactors hence provide an isobaric and isothermal environment free from transport limitations for the direct DME synthesis, in the kinetic regime as well as at equilibrium conversion.

14/02044 Compatibility of a post-industrial ceramic with nitrate molten salts for use as filler material in a thermocline storage system

Calvet, N. *et al. Applied Energy*, 2013, 109, 387–393.
This paper demonstrates the potential of a post-industrial ceramic commercially called Cofalit® as a promising, sustainable, and cheap filler material in a molten salt direct thermocline storage system. This ceramic, which comes from industrial treatment of asbestos containing waste, demonstrates relevant properties to store thermal energy by sensible heat up to 1100 °C and is very inexpensive. In this study, the compatibility of this ceramic with two different molten salts – the conventional binary solar salt and a promising ternary nitrate salt also called HITEC XL – is tested at medium temperature (500 °C) under static state. The objective is to develop a molten salt thermocline direct storage system using low-cost shaped ceramic as filler material. It should significantly decrease the cost of parabolic trough storage systems and simultaneously increase the efficiency of the plants by producing superheated steam at higher temperature.

14/02045 Economic and environmental analysis of a trigeneration system for food-industry: a case study

Freschi, F. *et al. Applied Energy*, 2013, 107, 157–172.
The application of a trigeneration system to fruit conservation food-industry is studied. The economic and environmental benefits of the installation are analysed by means of multi-objective optimization which takes into account operational costs of the system and greenhouse gas emissions. A contrast between the minimization of these two objectives is shown and thus different operative strategies are devised. Taken a practical case of the trigeneration load required by an industrial site in north-west of Italy where measurements of load profiles are available, different combined heat and power engines with and without a thermal energy storage system are studied and results are discussed. General considerations about the advantages of the proposed solutions are also presented.

14/02046 Energetic and exergetic analysis of waste heat recovery systems in the cement industry

Karellas, S. *et al. Energy*, 2013, 58, 147–156.
In a typical cement producing procedure, 25% of the total energy used is electricity and 75% is thermal energy. However, the process is characterized by significant heat losses mainly by the flue gases and the ambient air stream used for cooling down the clinker (about 35%–40% of the process heat loss). Approximately 26% of the heat input to the system is lost due to dust, clinker discharge, radiation and convection losses from the kiln and the preheaters. A heat recovery system could be used to increase the efficiency of the cement plant and thus contribute to emissions decrease. The aim of this paper is to examine

and compare energetically and exergetically, two different waste heat recovery (WHR) methods: a water-steam Rankine cycle, and an organic Rankine cycle (ORC). A parametric study proved that the water steam technology is more efficient than ORC in exhaust gases temperature higher than 310 °C. Finally a brief economic assessment of the most efficient solution was implemented. WHR installations in the cement industry can contribute significantly in the reduction of the electrical consumptions operating cost thus being a very attractive investment with a payback period up to 5 years.

14/02047 Energy use and CO_2 emissions of China's industrial sector from a global perspective

Zhou, S. *et al. Energy Policy*, 2013, 58, 284–294.

The industrial sector has accounted for more than 50% of China's final energy consumption in the past 30 years. Understanding the future emissions and emissions mitigation opportunities depends on proper characterization of the present-day industrial energy use, as well as industrial demand drivers and technological opportunities in the future. Traditionally, however, integrated assessment research has handled the industrial sector of China in a highly aggregate form. This study develops a technologically detailed, service-oriented representation of 11 industrial subsectors in China, and analyses a suite of scenarios of future industrial demand growth. It was found that, due to anticipated saturation of China's per capita demands of basic industrial goods, industrial energy demand and CO_2 emissions approach a plateau between 2030 and 2040, then decrease gradually. Still, without emissions mitigation policies, the industrial sector remains heavily reliant on coal, and therefore emissions-intensive. With carbon prices, it was observed that there was some degree of industrial sector electrification, deployment of CO_2 capture and storage at large industrial point sources of CO_2 emissions at low carbon prices, and an increase in the share of combined heating and power systems at industrial facilities. These technological responses amount to reductions of industrial emissions (including indirect emission from electricity) of 24% in 2050 and 66% in 2095.

14/02048 Evaluation of different hedging strategies for commodity price risks of industrial cogeneration plants

Palzer, A. *et al. Energy Policy*, 2013, 59, 143–160.

This study designs and evaluates eight different strategies for hedging commodity price risks of industrial cogeneration plants. Price developments are parameterized based on EEX data from 2008 to 2011. The probability distributions derived are used to determine the value-at-risk of the individual strategies, which are in a final step combined in a mean-variance portfolio analysis for determining the most efficient hedging strategy. It was found that the strategy adopted can have a marked influence on the remaining price risk. Quarter futures are found to be particularly well suited for reducing market price risk. In contrast, spot trading of CO_2 certificates is found to be preferable compared to forward market trading. Finally, portfolio optimization shows that a mix of various hedging strategies can further improve the profitability of a heat-based cogeneration plant.

14/02049 Exergy analyses in cement production applying waste fuel and mineralizer

Renó, M. L. G. *et al. Energy Conversion and Management*, 2013, 75, 98–104.

The cement industry is an energy-intensive industry and emits large quantities of carbon dioxide, so waste fuels could usefully substitute part of the fossil fuels. They can also help resolve air pollution problems associated with the use of fossil fuels. This study presents an exergy analysis of clinker production, a powerful tool which has been used in the performance evaluation of energy-related systems. The results indicate that the main irreversibility source in the cement industry is the rotary kiln and calciner process where the clinkerization process occurs. Therefore, the use of mineralizers and alternative fuels is important, especially for reducing the fossil fuel consumption (in this study the reduction was 17.32 t/day of fossil fuel) and waste management problems. However, it is necessary to take into account that the choice of alternative fuel depends on price and availability, and that the energy and ash contents are also important, as are the moisture and volatiles contents. This is a potential area for future research and development.

14/02050 Experimental study of steam methane reforming in a Pd-based fluidized bed membrane reactor

Roses, L. *et al. Chemical Engineering Journal*, 2013, 222, 307–320.

This work investigates the production of pure hydrogen by steam methane reforming in a fluidized bed membrane reactor. Hydrogen is separated though palladium based dense membranes from the products of steam methane reforming reaction in a fluidized bed containing a catalytic partial oxidation (CPO) catalyst. First, a 2-week run test was performed assessing the reactor stability during the whole test and the membrane perm-selectivity (H_2/other gases) remained 100% even operating at elevated temperatures (903 K) and under bubbling fluidization regime. As the reactor demonstrated to be reliable and the membrane stable for a long period, a parametric study has been carried out highlighting the reactor performances in terms of methane conversion and hydrogen permeation. Moreover, the deviation from ideal reactor operation is outlined by studying the approach to equilibrium conversion and its connections with operating conditions. The operating conditions tested varied in the 773–903 K temperature range and 2.0–5.3 bar reacting pressure. The effect of weight hourly space velocity, steam to carbon ratio and dilution of the reacting mixture with an inert gas on the reactor performance were also investigated. Experimental results show that higher temperatures and pressures have positive effect both on approach to equilibrium conversion and on hydrogen yield, while opposite effects arise from increasing steam to carbon ratio and weight hourly space velocity.

14/02051 Film cooling on a gas turbine blade suction side with converging slot-hole

Yao, Y. *et al. International Journal of Thermal Sciences*, 2013, 65, 267–279.

Experimental investigation was conducted in the current study to investigate the film cooling performance of a single row of consoles on a large-scale curved-plate model simulating the blade suction side, and an aided numerical study was also made to reveal the detailed film cooling features of consoles on the curved surface. A comparison in contrast to cylindrical hole was made. For the console cooling geometry, the interaction between coolant jet from inclined console and the mainstream flow results in reasonable vortices configuration to reduce mainstream–coolant interaction. And additional corner vortices are observed in the intersection of two consoles on the convex surface. The console row shows great potential in the blade film cooling application to produce high cooling effectiveness, especially at large blowing ratios. But this is at the expense of greater pressure drop. And the heat transfer coefficient ratio for the console is a little bigger than conventional cylindrical hole. Furthermore, the effects of major factors on the film cooling effectiveness, heat transfer coefficient and discharge coefficient were explored, including film hole location, blowing ratio and primary flow Reynolds number.

14/02052 Investigation of water droplet carryover phenomena in industrial evaporative air-conditioning systems

Koseoglu, M. F. *International Communications in Heat and Mass Transfer*, 2013, 47, 92–97.

Water droplet carryover phenomena and pressure drop characteristics in drip-type direct evaporative coolers have been experimentally investigated. Ten different evaporative cooling pads were tested for different air frontal velocities, and the onset of carryover has been determined. The onset of water carryover has been found to be at air velocities between 3.5 and 4.2 m/s. Also, the effect of flute height and pad thickness on pressure drop characteristics of cooling pads has been examined. In addition, it has been determined that for the steady-state operation of drip-type direct evaporative coolers, water temperature in the reservoir approaches the wet-bulb temperature and can be taken as constant for long-term steady-state operations in practice.

14/02053 Multicriteria optimization of a distributed energy supply system for an industrial area

Buoro, D. *et al. Energy*, 2013, 58, 128–137.

This paper presents a multi-objective optimization model for distributed energy supply systems optimization. The superstructure of the system comprehends a district heating network that connects the users to each other, small-scale combined heat and power systems, large centralized solar plant and a thermal storage. The optimization has to determine the optimal structure of the system, the size of each component inside the optimal solution and the optimal operation strategy. The multi-objective optimization is based on a mixed integer linear programming model and takes into account as objective function a linear combination of the annual cost for owning, maintaining and operating the whole system and the CO_2 emissions associated to the system operation. The model provides different optimal solutions by varying the relative weight of the economic and the environmental objectives. In this way the Pareto front is identified and the possible improvements in both economic and environmental terms can be highlighted. The model has been applied to a specific case study and it has been optimized for different superstructure configurations and for two different values of the electricity carbon intensity. The obtained results show that the solar plant, coupled with the optimal thermal storage, allows reaching both environmental and economic goals.

14/02054 Optimization of process integration in a Kraft pulp and paper mill – evaporation train and CHP system

Mesfun, S. and Toffolo, A. *Applied Energy*, 2013, 107, 98–110.

A great interest has been arising about the production of fuels and advanced chemicals from renewable resources such as wooden biomass in the so-called biorefineries. Pulp and paper mills are often seen as the

most obvious fundamental module of such industrial sites, because of the common feedstock and the chemical transformations that already occur in the process. In this paper the model of real Kraft pulp and paper mill is developed and optimized from energetic point of view using process integration techniques, in order to assess the potential for energy saving and to establish a starting point for future research on biorefinery sites. Improvements to the configurations of the multi-effect evaporator and of the steam cycle in the combined heat and power system have been introduced, and three different levels of heat integration boundaries have been considered (multi-effect evaporator, mill sub-processes, and total site). Results indicate a significant potential for the decrease in thermal energy requirement and/or the increase in power production for the same pulp and paper production.

14/02055 Oversizing analysis in plant-wide control design for industrial processes
Zumoffen, D. A. R. *Computers & Chemical Engineering*, 2013, 59, 145–155.
In this work, an alternative plant-wide control design approach based on oversizing analysis is presented. The overall strategy can be divided in two main sequential tasks: (1) defining the optimal decentralized control structure, and (2) setting the controller interaction degree and its implementation. Both problems represent combinatorial optimizations based on multi-objective functional costs and were solved efficiently by genetic algorithms. The first task defines the optimal selection of controlled and manipulated variables simultaneously, the input–output pairing, and the overall controller dimension in a sum of square deviations context. The second task analyses the potential improvements by defining the controller interaction degree via the net load evaluation approach. In addition, some insights are given about the feasibility (implementation load) of these control structures for a decentralized or centralized framework. The well-known Tennessee Eastman process is selected here for sake of comparison with other multivariable control designs.

14/02056 Post-combustion capture of CO_2 at an integrated steel mill – part I: technical concept analysis
Arasto, A. *et al. International Journal of Greenhouse Gas Control*, 2013, 16, 271–277.
In this study different possibilities for applying post-combustion capture at an integrated steel mill in order to reduce carbon dioxide emissions were studied. Implications of different amounts of CO_2 captured, different solvents for post-combustion capture and different heat supply options for solvent regeneration to the energy balance and greenhouse gas emissions of the steel mill are compared to that of the base case for the steel mill. The case study is based on Ruukki Metals' Raahe steel mill that is situated on the coast of the Gulf of Bothnia. It is the largest integrated steel mill in the Nordic countries producing hot rolled steel plates and coils. It is also the largest CO_2 point source in Finland emitting approximately 4 Mt/year. Carbon capture processes were modelled using Aspen Plus process modelling software and results were used to estimate the potential for reducing CO_2 emissions at an integrated steel mill from a plant operator's point of view. Different heat integration options and heat utilization scenarios were investigated. The heat available for solvent regeneration varied between these heat utilization scenarios and thus partial capture of CO_2 was investigated with the CO_2 amount captured depending on the heat available for solvent regeneration in the different case studies. The results of the study show a significant CO_2 reduction potential using CCS. Approximately 50–75% of the emissions from the site could be captured using post-combustion capture. Capturing a larger amount of emissions would be technically less feasible due to the large number of small stacks around the large, integrated steel mill site.

14/02057 Post-combustion capture of CO_2 at an integrated steel mill – part II: economic feasibility
Tsupari, E. *et al. International Journal of Greenhouse Gas Control*, 2013, 16, 278–286.
In this paper, the economics of the technical possibilities presented in the first part of this study for applying post-combustion CO_2 capture at an integrated steel mill were studied. Implications of different CO_2 amounts captured, solvents and process integration levels to the greenhouse gas balances and economics of operation are compared to the reference case without CO_2 capture and storage (CCS) trough several case studies using variable market prices of electricity and CO_2 emission allowances. The break-even price (BEP) of CO_2 emissions (e.g. CO_2 emission allowances), where CCS becomes more profitable than the reference case, is about 72 €/t CO_2 with an electricity price of 100 €/MWh in the most favourable studied case using a MEA solvent. For the more advanced solvents considered, the BEP level is about 64 €/t CO_2. With higher prices of electricity, the costs for CCS increase rapidly. The costs for globally avoided emissions, based on a streamlined life-cycle analysis, are generally higher than the BEP's, depending on the fuels that are assumed to eventually compensate the decreased electricity production in the energy system. The amounts of captured CO_2 corresponding to the above presented prices in the most favourable cases are typically in the range of 2–3 Mt CO_2/a, which accounts for 50–75% of the site emissions.

14/02058 Strategic energy management in the primary aluminium industry: self-generation as a competitive factor
Lucio, N. R. *et al. Energy Policy*, 2013, 59, 182–188.
The Brazilian aluminium industry, classified as energy-intensive, consumes alone about 6% of all power generated by hydro-electric power plants, and therein lies much of the problem: needs lots of energy to produce primary aluminium. The aim of this study is to evaluate the strategy of energy self-generation as a viable alternative of sustainable growth and its importance for the competitive primary aluminium industry in Brazil and outlines key tactics to self-generation adopted for different economic scenarios and conditions in which it would be effective. Also environmental aspects are considered because their impacts in costs and the impact of recycling in the environment through, mainly, reuse of aluminium from cans. Given the instability of energy prices on the open market and supply volatility, self-generation appears as the best alternative for maintaining the sustainability of the primary aluminium industry in Brazil.

14/02059 The status of energy conservation in Taiwan's cement industry
Su, T.-L. *et al. Energy Policy*, 2013, 60, 481–486.
The cement industry represents one of the most energy-intensive sectors in Taiwan. Energy audits are the direct tools which are employed to help reduce energy consumption. The objectives of energy audits are to establish energy audit systems, provide on-site energy audit service and reduce production cost. This study summarized the energy savings implemented in Taiwan's cement industry; the data were obtained from the on-line energy declaration system in 2010. The total implemented energy savings amounted to 68,512 kilolitres of crude oil equivalent (KLOE). The energy audit group audited seven Taiwanese cement plants in 2011 and revealed an energy saving potential of 2571.6 MWh of electricity and 1002.8 KLOE of thermal energy. The total potential energy saving was 1708.5 KL of crude oil equivalent (KLOE), equivalent to a 4560 t reduction in CO_2 emissions, representing the annual CO_2 absorption capacity of a 122 ha forest plantation.

14/02060 Toward integrated production and distribution management in multi-echelon supply chains
Cóccola, M. E. *et al. Computers & Chemical Engineering*, 2013, 57, 78–94.
The effective management of multi-site systems involves the proper coordination of activities performed in multiple factories, distribution centres, retailers and end-users located in many different cities, countries and/or continents. To optimally manage numerous production and transportation decisions, a novel monolithic continuous-time mixed integer linear programming-based framework is developed to determine the best short-term operational planning to meet all customer requests at minimum total cost. The formulation lies on the unit-specific general precedence concept for the production scheduling problem whereas the immediate precedence notion is used for transportation decisions. To illustrate the applicability and potential benefits of the model, a challenging example corresponding to a supply chain comprising several locations geographically spread in six European countries has been solved to optimality with modest computer process times. Several scenarios with different logistics features were addressed in order to remark the significant advantages of using the integrated approach.

10 SPACE HEATING AND COOLING/HEAT PUMPS

14/02061 A building thermal bridges sensitivity analysis
Capozzoli, A. *et al. Applied Energy*, 2013, 107, 229–243.
As the new European Directive 2010/31/EU on the Energy Performance of Buildings (EPBD recast) comes into force, each European Union (EU) member state has the responsibility of supporting activities for the construction of nearly zero-energy buildings with a very high energy performance. In order to achieve the new EU directive targets, designers, in addition to having to use innovative building components, also have to pay more attention to the construction details that affect building envelope heat losses. It is therefore necessary not only to properly design structural nodes, in order to minimize such energy losses, but also to identify accurate numerical methods in order to appreciate the benefits of a proper design. A sensitivity analysis based on an extensive study of the linear

thermal transmittance value of many types of thermal bridge, based on the methodology specified in EN ISO 10211, has been carried out in the presented work. After having defined the input design variables and considering a range of variation for each of them for the linear thermal transmittance evaluation, a non-linear regression model has been specifically developed for each analysed thermal bridge, considering the output values of a numerical code as data set. In order to perform the sensitivity analysis a significant and representative number of cases have been generated, using a sampling technique. The ANOVA–FAST method has been performed, on the basis of the obtained results, in order to assess the contribution of each input design variable to the deviation of the linear thermal transmittance for each kind of thermal bridge.

14/02062 A general exact solution for heat conduction in multilayer spherical composite laminates

Norouzi, M. *et al. Composite Structures*, 2013, 106, 288–295.

In this study, an exact analytical solution for steady conductive heat transfer in multilayer spherical fibre-reinforced composite laminates is presented for the first time. Here, the orthotropic temperature distribution of laminate is obtained under the general linear boundary conditions that are suitable for various conditions including combinations of conduction, convection, and radiation both inside and outside of the sphere. The temperature and heat flux continuity is applied between the laminas. In order to obtain the exact solution, the separation of variables method is used and the set of equations related to the coefficient of Fourier–Legendre series of temperature distribution is solved using the recursive Thomas algorithm. The capability of the present solution is examined by applying it on two industrial applications for different fibre arrangements of multilayer spherical laminates.

14/02063 A mixed-gas miniature Joule–Thomson cooling system

Derking, J. H. *et al. Cryogenics*, 2013, 57, 26–30.

A mixed-gas Joule–Thomson (JT) cooling system is investigated in which a micromachined JT cold stage of $60 \times 10 \times 0.7\,mm^3$ is combined with a linear compressor. The cooling system is operated between 1.3 and 9.4 bar with a ternary gas mixture of 39 mol% methane, 20 mol% ethane and 41 mol% isobutane. It cools down to below 130 K, and at a cold-tip temperature of 150 K, a cooling power of 46 mW is obtained at a mass-flow rate of $1.35\,mg\,s^{-1}$. The background losses are experimentally determined to be 20 mW and are in good agreement with the calculated value of 21 mW. The linear compressor can be used to drive 19 of these miniature JT cold stages in parallel, e.g. for cooling optical detectors in future space missions. In this mode, the compressor pressure ratio is slightly less, resulting in a net cooling power of 23 mW per miniature JT cold stage.

14/02064 A non-Gaussian pattern matching based dynamic process monitoring approach and its application to cryogenic air separation process

Chen, J. *et al. Computers & Chemical Engineering*, 2013, 58, 40–53.

Principal component analysis (PCA)-based pattern matching methods have been applied to process monitoring and fault detection. However, the conventional pattern matching approaches do not specifically take into account the non-Gaussian dynamic features in chemical processes. Furthermore, those techniques are more focused on fault detection instead of fault diagnosis. In this study, a non-Gaussian pattern matching based fault detection and diagnosis method is developed and applied to monitor cryogenic air separation process. First, independent component analysis (ICA) models are built on the normal benchmark and monitored data sets along sliding windows. The IC subspaces from the benchmark and monitored data are then extracted to evaluate the non-Gaussian patterns and detect process faults through a mutual information based dissimilarity index. Further, a difference subspace between the two IC subspaces is computed to characterize the divergence of the dynamic and non-Gaussian patterns between the benchmark and monitored data. Subsequently, the mutual information between the IC difference subspace and each process variable direction is defined as a new non-Gaussian contribution index for fault identification and diagnosis. The presented approach is applied to a simulated cryogenic air separation plant and the monitoring results are compared against those of PCA-based pattern matching techniques and ICA-based monitoring method. The application study demonstrates that the developed non-Gaussian pattern matching approach can effectively monitor the complex air separation process with superior fault detection and diagnosis capability.

14/02065 A numerical and experimental investigation on microscale heat transfer effect in the combined entry region in macro geometries

Kong, K. S. and Ooi, K. T. *International Journal of Thermal Sciences*, 2013, 68, 8–19.

The rising heat dissipation problem in electronic devices has led to numerous investigations on microchannel heat sink. However, literature shows that microscale heat transfer is generally not being applied to macro geometries, which is believed largely due to the fabrication and operational challenges. In the present study, experiments were conducted in a conventionally-sized circular channel which was manufactured through conventional techniques. The channel has a nominal diameter of 20 mm and length of 30 mm. An insert was placed concentrically into the channel to make the flow path small enough to behave like a microchannel in order to attain high heat removal capabilities. Under such a construction, various sizes of channel can be formed by placing different sizes of insert, one at a time, into the circular channel. The experiments and numerical simulations were conducted for nominal gap sizes of 1000 and 300 μm over a range of Reynolds numbers from 1000 to 5500 and heat fluxes from 5.3 to $37.1\,W/cm^2$ in the combined entry region. The experimental findings showed that the design was able to achieve a maximum heat transfer coefficient of $68\,kW/m^2\,K$ with single-phase water flowing through the annular channel of gap size of 300 μm at Reynolds number of 5200. Comparisons of measurements from the 300-μm case with the numerical solutions showed good agreement for pressure drop predictions with an average deviation of 4.5% but poor agreement for the Nusselt number predictions with deviation of more than 30% for cases at higher Reynolds number. Most importantly, the experiments have demonstrated the possibility of achieving microscale heat transfer effects in macro geometries using readily available conventional fabrication methods. With microscale heat transfer effects easily available, it also presents an opportunity to effectively improve the heat removal capabilities of a macroscale heat exchanger in the near future.

14/02066 A statistical analysis on market-available solar thermal heat pump systems

Ruschenburg, J. *et al. Solar Energy*, 2013, 95, 79–89.

During the past few years, many combined solar thermal heat pump systems have entered the residential heating and/or domestic hot water generation market. In order to determine the suitability of currently developed methods for testing or assessing such systems for present-day solutions, a thorough review and analysis of market-available systems are essential. The basis of the presented analysis is formed by 135 combined solar thermal heat pump systems that were researched and documented from October 2011 to September 2012. They were provided by 88 companies from 11 countries. The characteristics of solar collectors and heat pumps are broken down at the component level. At the system level, the characterization is centred on the interaction between solar collectors and heat pump. Here, numerous reviewed systems follow concepts using solar thermal energy as a low-temperature energy source for the heat pump, either additionally or exclusively. It is shown by cross analysis that this feature applies especially to systems incorporating unglazed collectors or photovoltaic-thermal collectors. More findings specific to the combination between collectors and heat pump, to climates or countries are presented as well. This research indicates that many solar thermal heat pump systems differ from standard concepts in various ways. The outcome motivates a holistic approach regarding testing and assessing of such systems.

14/02067 Active free cooling optimization with thermal energy storage in Stockholm

Chiu, J. N. W. *et al. Applied Energy*, 2013, 109, 523–529.

Latent heat thermal energy storage (LHTES) integrated active free cooling stores night time cold and serves as heat sink for cooling when demand rises. Passive buildings, albeit their advantages in limiting heat loss during winter time, are often paired with excessive internal overheating in summer, as shown in the first part of this study. Under the climate condition in Stockholm, LHTES systems may provide solutions for sustainable cooling with use of renewable cooling sources. This study presents a multi-objective optimization on system cost and cooling supply for various LHTES configurations followed with a sensitivity analysis on phase change material cost and energy price. Results indicate that optimized LHTES may meet cooling needs while retaining economic viability. However, LHTES based cooling systems may require substantially higher electricity demand than conventional air conditioning unit for applications where high cooling thermal power rate is to be met, a trade-off to indoor comfort level needs to be considered to reach the concept of sustainable free cooling. This study provides a novel techno-economic feasibility study of active free cooling LHTES in Stockholm as well as new insights to cost, comfort level and energy requirement with use of multi-objective optimization algorithm.

14/02068 An investigation in the effects of recycles on laminar heat transfer enhancement of parallel-flow heat exchangers

You, Y. *et al. Chemical Engineering and Processing: Process Intensification*, 2013, 70, 27–36.

It was demonstrated that fluid recycling could effectively enhance heat transfer rates of heat exchangers, however, related investigations were limited. In the current work, parallel-flow heat exchangers with basic recycles or revised recycles are investigated in the laminar regime. Theoretical models of thermo-hydraulic performances are established. The effects of reflux ratio, capacitance rate ratio, heat transfer area, and recycle length are investigated. The results demonstrate that the dimensionless heat transfer rate rises with the increase of reflux ratio or capacitance rate ratio, or with the decrease of heat transfer area, and the maximum values reach up to 127% and 121% for basic internal and external recycles, respectively. Basic internal recycles generate larger dimensionless heat transfer rates under larger reflux ratios, while basic external recycles perform more reliably over the whole reflux ratio range. Compared with basic recycles, revised recycles (i.e. partial-length recycles) require smaller pumping powers. Thus, partial-length recycles can improve the dimensionless overall performance of full-length recycle heat exchangers, e.g. half-length recycles increase the dimensionless overall performance by 65%. Fluid recycling does not need to change geometrical structures and fluid flow rates, thus it is a competitive approach of thermal augmentation in heat exchangers.

14/02069 Analysis of the hot-disk technique applied to low-density insulating materials

Coquard, R. *et al. International Journal of Thermal Sciences*, 2013, 65, 242–253.

The hot-disk technique is a very practicable transient method of measurement of the thermal properties of solid materials. It has been applied successfully to a wide variety of materials. However, it is based on several approximations regarding the nature of the heat transfer. Notably, the probe is considered thermally neutral, and the heat transfer is assumed purely conductive. These two assumptions are questionable when dealing with low-density thermal insulators. In order to evaluate the accuracy of the method, the authors have generated numerically noised thermograms reproducing the thermal response that would be recorded when measurements are applied to those type of materials. Thereafter, the best-fitting procedure of the classical hot-disk technique was applied to these thermograms. The analysis of the identification results show that the presence of a radiative contribution do not affect the accuracy of the thermal properties identified. The conductivity measured actually corresponds to the equivalent conductivity. On the other hand, when the method is applied to materials with thermal inertia strongly different from the probe (about two orders of magnitude lower or more), the accuracy of the method becomes questionable. This is notably the case for common insulators used in the building industry like polymer foam or mineral wools. The preceding conclusions have been validated by experimental measurements on a standard low-density extruded polystyrene foam sample and a superinsulating silica aerogel.

14/02070 Cross-flow heat exchangers for anti-freezing of liquid nitrogen

Chang, H.-M. *et al. Cryogenics*, 2013, 57, 122–128.

Cross-flow heat exchangers are proposed and experimentally investigated as an anti-freezing scheme of liquid nitrogen. The possibility of freeze-out of liquid nitrogen is an important design issue in developing long superconducting cables, as the supply temperature of liquid nitrogen is close to its freezing temperature (63.3 K). Plate-fin heat exchangers are fabricated as typical counter-flow and newly proposed two-pass cross-flow in laboratory scale, and tested with cold helium gas at temperatures below 60 K. The experimental results show that the cross-flow heat exchanger is less vulnerable to the freeze-out condition, since the temperature distribution is basically two-dimensional. The cross-flow heat exchangers are effective in avoiding a complete clog-up of all passages and reducing the risk of freeze-out of liquid nitrogen.

14/02071 Design and performance of a solar air heater with long term heat storage

Saxena, A. *et al. International Journal of Heat and Mass Transfer*, 2013, 60, 8–16.

Solar air heaters are used for applications at low and moderate temperatures such as; crop drying, timber seasoning, and space heating. In the present work efforts are made to enhance the heat transfer rate and to improve the efficiency of simple fabricated solar air heater. 'Granular carbon', has introduced as a long-term heat absorbing media inside solar heater. The thermal performance evaluation of solar heater has been carried out on four different configurations by operating it on natural and forced convection. The thermal behaviour of the system has also been evaluated by operating it on auxiliary power by placing a halogen tube (300 W) inside the inlet and outlet ducts. Because of using halogen lights the system is feasible to perform in night or bad climatic conditions. The thermal performance of all new configurations was found better in comparison of conventional solar air heater on both natural and forced convection.

14/02072 Development of phase change materials for building applications

Sharma, A. *et al. Energy and Buildings*, 2013, 64, 403–407.

This paper deals with the development of eutectics based on commercial grade fatty acids, i.e. capric acid (CA), lauric acid (LA), myristic acid (MA), palmitic acid (PA) and stearic acid (SA), which are used as a form-stable, solid–liquid phase change materials (PCM) for thermal energy storage and with determination of their thermal properties. In this regard, a series of eutectics, i.e. CA–LA, CA–MA, CA–PA and CA–SA developed with different weight percentages (10/90, 20/80, 30/70, 40/60, 50/50, 60/40, 70/30, 80/20 and 90/10). Thermal characteristics such as melting temperature and latent heat of fusion of these developed eutectics measured by using differential scanning calorimetry (DSC), which also showed that developed eutectics were good candidates for building applications in terms of their large latent heat values and suitable phase change temperatures. The DSC results also showed that the melting temperatures and latent heat values of the developed PCMs are in the range of about 20–30 °C and 100–160 J/g. It was also found that CA weight percentage has a significant role in the melting temperature of developed tactics.

14/02073 Distillation assisted heat pump in a trichlorosilane purification process

Díez, E. *et al. Chemical Engineering and Processing: Process Intensification*, 2013, 69, 70–76.

The objective of this paper is to design and optimize a trichlorosilane distillation system with the aim of obtaining this product with a purity higher than 0.99999 mole fraction, so that it can employed as a source of solar-grade silicon. A conventional process with at least two columns is capable of separating the trichlorosilane from a mixture of this compound with dichlorosilane and silicon tetrachloride; however, due to the high purity required, large reflux ratios are needed. For this reason, a vapour recompression heat pump was considered for both columns but also for the second column only. All the alternatives were simulated with HYSYS® software platform, in order to determine economically the best one. The economic analysis indicates that, although in both heat pump assisted systems, the initial investment should be much larger than in the conventional process, the annual savings (29% for the double heat pump assisted system and 4% for the single heat pump assisted system), justify the use of heat pumps instead of traditional reboiler–condenser columns.

14/02074 Effect of component layout on the operation of a miniature cryogenic loop heat pipe

Bai, L. *et al. International Journal of Heat and Mass Transfer*, 2013, 60, 61–68.

Cryogenic loop heat pipes (CLHPs) are effective and efficient cryogenic heat transport devices suitable for many space and terrestrial applications. Due to the complexity of its structure, the start-up and operation of CLHPs might be influenced by the relative position of different components; however, little work has been done on this aspect. In this work, a miniature CLHP with nitrogen as the working fluid employing an auxiliary loop to assist the supercritical start-up was developed. The effect of the layout of the secondary loop line and the gas reservoir on the start-up and operation of the CLHP was experimentally investigated. The experimental results show that the relative position of these components can affect both the start-up and steady-state operation of the CLHP. The heat transport capacity of the CLHP can be increased considerably when the secondary loop line is connected to the middle or top of the primary compensation chamber.

14/02075 Effect of d-mannitol polymorphism in its thermal energy storage capacity when it is used as PCM

Barreneche, C. *et al. Solar Energy*, 2013, 94, 344–351.

The main objective of this paper is to study the possible use of d-mannitol as phase change material (PCM) for thermal energy storage. PCM are materials that have high-phase change enthalpy and this thermophysical property gives them the ability to store energy as latent heat. d-Mannitol is a material which has different morphological phases (polymorphism); here were studied β-form and δ-form. Different polymorphic forms produce changes on melting point of d-mannitol. For this reason it is necessary to establish a suitable working temperature range for the use of d-mannitol as phase change material. The thermal characterization was performed with DSC analysis using 0.5 K min^{-1} slow-dynamic method. Polymorphism analysis of d-mannitol was analysed to associate the thermal behaviour obtained by differential scanning calorimetry (DSC) with a specific polymorphic phase. d-Mannitol presented three different thermal behaviours: the first one had a melting peak at 167 °C, the second was a double melting peak at 155 °C and 166 °C, and the third a single peak at 155 °C. Due to irregular results, two working range were studied and through the thermal characterization, it was possible to define a working range where d-mannitol could be used as PCM for energy storage: this range is between 135 and 175 °C. Furthermore, it was possible to differentiate

two crystalline phases of d-mannitol applying Fourier transform infrared spectroscopy analysis and to link them with thermal behaviour observed in DSC. The percentage of times each thermal behaviour is observed in DSC analysis was calculated. δ-form is obtained 15.8% of analysed cycles, the β-form appears 44.7% of times, and an intermediate transition between the two phases is found 39.5% of cycles.

14/02076 Efficient cooling energy supply with aquifer thermal energy storages

Kranz, S. and Frick, S. *Applied Energy*, 2013, 109, 321–327.

Within this paper, the characteristics of aquifer thermal energy storage (ATES) for building cooling are discussed for the example of an existing ATES, which has been used for the cooling of the German Parliament buildings for almost 10 years. Based on the analysis of measurement data, it will be shown that the studied system has reached a coefficient of performance (COP) of between 3.6 and 7.8 over the time period considered. Based on the results of numerical simulations it will be shown that the COP can be even increased. Choosing proper operating conditions and design parameters, such as the temperature level of the cooling network or the regeneration temperature of the ATES, the efficiency of both, the studied system and future ATES projects, can be increased remarkably.

14/02077 Entropy generation analysis of an adsorption cooling cycle

Thu, K. *et al. International Journal of Heat and Mass Transfer*, 2013, 60, 143–155.

This paper discusses the analysis of an adsorption (AD) chiller using system entropy generation as a thermodynamic framework for evaluating total dissipative losses that occurred in a batch-operated AD cycle. The study focuses on an adsorption cycle operating at heat source temperatures ranging from 60 to 85 °C, whilst the chilled water inlet temperature is fixed at 12.5 °C – a temperature of chilled water deemed useful for dehumidification and cooling. The total entropy generation model examines the processes of key components of the AD chiller such as the heat and mass transfer, flushing and de-superheating of liquid refrigerant. The following key findings are observed: (i) the cycle entropy generation increases with the increase in the heat source temperature (10.8–46.2 W/K) and the largest share of entropy generation or rate of energy dissipation occurs at the adsorption process, (ii) the second highest energy rate dissipation is the desorption process, and (iii) the remaining energy dissipation rates are the evaporation and condensation processes, respectively. Some of the noteworthy highlights from the study are the inevitable but significant dissipative losses found in switching processes of adsorption–desorption and vice versa, as well as the de-superheating of warm condensate that is refluxed at non-thermal equilibrium conditions from the condenser to the evaporator for the completion of the refrigeration cycle.

14/02078 Evaluation of overall thermal transfer value (OTTV) for commercial buildings constructed with green roof

Chan, A. L. S. and Chow, T. T. *Applied Energy*, 2013, 107, 10–24.

Overall thermal transfer value (OTTV) is a measure of average heat gain into a building through the building envelope. It is a widely adopted measure in many countries for enhancing energy-efficient building design. In the past decade, there is increasing application of green roof into commercial buildings for enhanced building insulation, leading to reduction in heat gain through the roof area as well as cooling requirement of a building. Since the current OTTV equations and coefficients were originally developed for buildings with traditional bare roof construction, building designers have difficulty to compute the OTTV for buildings constructed with green roofs. The aim of this study is to revise the existing OTTV calculation method and derive a set of correction factors for OTTV evaluation of green roof integrated buildings. An experimental setup of a green roof system with sensors was installed on the rooftop of a commercial building. The measured data were used for validation of a building energy simulation program EnergyPlus incorporated with a green roof model Ecoroof. Four building cases with typical and traditional roof constructions were modelled using the validated computer simulation program. Through a series of parametric computer simulations, a correlation between OTTV and annual heat gain through the roof area was established with that a set of correction factors ranging from 0.03 to 0.99 was developed. These correction factors can be used by building designers to compute the OTTV of green roofs constructed on the rooftop of a commercial building, reflecting the thermal insulation capacity of substrate layers and vegetation plant in a green roof system. Although the methodology of this study was adopted for subtropical Hong Kong, it is envisaged that this approach could be applied to other locations with different climatic conditions to derive appropriate correction factors for OTTV evaluation of green roof integrated buildings.

14/02079 Improving dryer energy efficiency and controllability simultaneously by process modification

Atuonwu, J. C. *et al. Computers & Chemical Engineering*, 2013, 59, 138–144.

This work establishes a relationship between dryer energy performance and controllability using energy balances and process resiliency analysis. It is shown that using the process gain matrix, the dryer energy efficiency can be reliably calculated with conditions for simultaneous controllability improvement established. By incorporating a drying rate modifying system such as a desiccant dehumidifier as an add-on, these conditions are shown to be achievable due to the extra dehumidification which can be manipulated using the additional degrees of freedom introduced by the sorption system. Due to the adsorbent regulation properties which are enhanced by high-temperature regeneration, the resilience of energy performance to disturbances is significantly improved compared to conventional dryers. Also, a desiccant system performance indicator, the adsorber–regenerator net energy efficiency (ARNEE) is introduced and it is shown that energy efficiency improvement is possible only if the ARNEE is greater than the energy efficiency of the stand-alone dryer.

14/02080 Integration of thermal insulation coating and moving-air-cavity in a cool roof system for attic temperature reduction

Yew, M. C. *et al. Energy Conversion and Management*, 2013, 75, 241–248.

Cool roof systems play a significant role in enhancing the comfort level of occupants by reducing the attic temperature of the building. Heat transmission through the roof can be reduced by applying thermal insulation coating (TIC) on the roof and/or installing insulation under the roof of the attic. This paper focuses on a TIC integrated with a series of aluminium tubes that are installed on the underside of the metal roof. In this study, the recycled aluminium cans were arranged into tubes that act as a moving-air-cavity (MAC). The TIC was formulated using titanium dioxide pigment with chicken eggshell waste as bio-filler bound together by a polyurethane resin binder. The thermal conductivity of the thermal insulation paint was measured using KD2 Pro Thermal Properties Analyser. Four types of cool roof systems were designed and the performances were evaluated. The experimental works were carried out indoors by using halogen light bulbs followed by comparison of the roof and attic temperatures. The temperature of the surrounding air during testing was approximately 27.5 °C. The cool roof that incorporated both TIC and MAC with opened attic inlet showed a significant improvement with a reduction of up to 13 °C (from 42.4 to 29.6 °C) in the attic temperature compared to the conventional roof system. The significant difference in the results is due to the low thermal conductivity of the thermal insulation paint (0.107 W/mK) as well as the usage of aluminium tubes in the roof cavity that was able to transfer heat efficiently.

14/02081 Mathematical modeling of a PCM storage tank in a solar cooling plant

Gallego, A. J. *et al. Solar Energy*, 2013, 93, 1–10.

Solar cooling plants can work in multiple operation modes. A numerical model of the whole plant can be used to choose the adequate operation mode and optimizing the energy production by using hierarchical control strategies. Simplified models are required for solving the control problem in a suitable time-window using systems such as programmable logic controllers or microcontrollers. The storage system is an important component of a solar cooling plant. They are useful in solar systems for helping to satisfy the energy demand when solar energy is not available. Those based on phase change materials (PCMs) have the advantage of high storage density at a small temperature range. This paper presents a simplified model of a PCM storage tank placed at the solar cooling plant of the Escuela Superior de Ingenieros in Seville, Spain, focusing on the parameter estimation algorithm.

14/02082 New highly efficient regeneration process for thermochemical energy storage

Mette, B. *et al. Applied Energy*, 2013, 109, 352–359.

Thermochemical energy storage is a key technology to realize highly efficient thermal energy storages for various applications such as solar thermal systems or cogeneration systems. As thermal storage material zeolite and composite materials of zeolite and salts, for example, are the subject of intensive research at present. These materials meet the combined requirements of high energy storage density and good heat transfer rates. However, in order to obtain a high energy storage density, comparatively high temperatures of in excess of 180 °C are needed during the regeneration process. This is a drawback especially when used as storage material in solar thermal systems. In this paper, a new regeneration strategy is proposed for an open sorption process. The new regeneration strategy allows regeneration of the storage material at significantly lower temperatures without reducing the energy storage density of the material. For the example of a solar

thermal combisystem with thermochemical energy storage, a concept for integrating this new regeneration strategy into an overall system will be presented. For an energetic assessment, annual system simulations have been performed with the dynamic simulation software TRNSYS. A comparison of the system design with a 'conventional' regeneration strategy (regeneration temperature of 180 °C) and with the new regeneration strategy (regeneration temperature of 130 °C) has been made. The results of the simulation study show that with the new regeneration strategy the fractional energy saving as a measure of the thermal performance of the system can be maintained or even increased. These promising results demonstrate that this process design may be a breakthrough in realizing thermochemical energy storages for solar thermal applications based on high performance zeolite or zeolite composite materials.

14/02083 New model to evaluate the effective thermal conductivity of three-phase soils

Gori, F. and Corasaniti, S. *International Communications in Heat and Mass Transfer*, 2013, 47, 1–6.

The aim of the present paper is to present a new model without empirical constants to evaluate the effective thermal conductivity of three-phase soils. In the model the soil is made of a quasi-spherical solid grain, and is surrounded by two phases, which can be air and water or air and ice. The effective thermal conductivity is obtained theoretically by the integration of the steady-state heat conduction equation under the thermal assumption of parallel heat fluxes. This new model allows one to evaluate the effective thermal conductivity of soils with porosity (ratio between the volume of the voids and the total one) in the range between 0.0349 and 0.4734 at all degrees of saturation (ratio between the water volume and the void one) from dryness up to saturation. Comparisons with experimental data of unfrozen and frozen soils confirm that the model can predict the effective thermal conductivity with a fairly good agreement without using any empirical constant.

14/02084 Numerical analysis of heat transfer in unglazed transpired collectors based on field synergy principle

Gao, L. *et al. Solar Energy*, 2013, 95, 336–344.

Numerical simulations were performed on heat transfer characteristics in an unglazed transpired collector (UTC) and a glazed flat-plate collector. The simulation results were analysed from the viewpoint of field synergy principle. It is found that velocity and temperature gradient are almost parallel to each other over most part of the computational domain in UTC, while nearly perpendicular to each other in glazed flat-plate collector. The average intersection angle between velocity vector and temperature gradient is 42.70° and 88.53° in UTC and glazed flat-plate collector, respectively. Heat transfer is significantly enhanced in UTC due to good synergy between velocity vector and temperature gradient, and the thermal efficiency of UTC is therefore much higher than that of glazed flat-plate collector. Field synergy principle could explain well the mechanism of heat transfer enhancement in UTC. Heat transfer in UTC is enhanced moderately with increasing suction velocity. The average intersection angle in UTC decreases with increasing suction velocity, rapidly at suction velocities below 0.05 m/s and slightly at suction velocities above 0.05 m/s. The effect of hole pitch on heat transfer in UTC is significant, while the effect of hole diameter is less pronounced.

14/02085 Performance study of parallel-type hybrid-power gas engine-driven heat pump system

Wang, Y. *et al. Energy and Buildings*, 2013, 62, 37–44.

This paper analyses the operating principle and the advantages of the parallel-type hybrid-power gas engine-driven heat pump system (PHGHP) and builds test systems to test the performance of the system in the heating conditions and cooling conditions. The PHGHP used the heat pump system's cooling capacity, heat capacity, fuel-consumed flow, fuel consumed-rate, thermal efficiency and reclaimed heat as the economic analysis parameters. In addition, this paper puts forward the concept of the equivalent fuel-consumed flow and the equivalent output power of engine. The test results show, the speed and torque of gas engines which used the baseline control strategy and combined with a gas engine optimization curve control strategy are always in the designated economic. Fuel-consumed flow changes in 280–340 g (kW h)$^{-1}$. With compressor speed increasing, the drive system thermal efficiency is maintained between 0.23 and 0.28.

14/02086 Pilot experimental study on shell and tube heat exchangers with small-angles helical baffles

Zhang, L. *et al. Chemical Engineering and Processing: Process Intensification*, 2013, 69, 112–118.

In this paper, the experimental comparisons of shell side thermodynamic and hydraulics performance are made among three helical baffles heat exchangers and one segmental baffles heat exchanger. The experiment scale is larger than the previous experimental setup as the diameter of test heat exchangers are 500 mm and the effective tube length are 6 m; the experiment mainly focuses on the small helical angle scheme as the helical angle ranges from 7° to 25°. Among all the four heat exchangers, both the shell side heat transfer rate and the shell side pressure drop peak when helical angle equals 7°, and the shell side heat transfer rate per unit pressure drop at this angle is the smallest. This phenomenon could be easily illustrated as the concept 'fluid-flow distance' is presented. At last, the correlations for the shell side Nusselt number and friction factor are presented as a reference.

14/02087 Preparation and characteristics of microencapsulated stearic acid as composite thermal energy storage material in buildings

Chen, Z. *et al. Energy and Buildings*, 2013, 62, 469–474.

Microencapsulated stearic acid (SA) with silicon dioxide (SiO_2) shell as composite thermal energy storage material was prepared using sol–gel methods. In the composite thermal energy storage material, the stearic acid was used as the core material that is the latent heat storage phase change material (PCM), and the silicon dioxide acted as the shell material which prevented the leakage of the melted stearic acid. Fourier transformation infrared spectroscopy and scanning electronic microscopy (SEM) were used to determine chemical structure and microstructure of microencapsulated stearic acid with silicon dioxide shell. The thermal properties and thermal stability were investigated by the differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). The SEM results showed that the stearic acid was encapsulated in the shell of the silicon dioxide shell. The DSC results indicated that the microencapsulated stearic acid with the silicon dioxide shell as composite thermal energy storage material solidifies at 52.6 °C with a latent heat of 162.0 kJ/kg and melts at 53.5 °C with a latent heat of 171.0 kJ/kg when the encapsulation ratio of the SA is 90.7%. The TGA results presented that the silicon dioxide shells can improve the thermal stability of the microencapsulated stearic acid as composite thermal energy storage material.

14/02088 Preparation and properties of highly conductive palmitic acid/graphene oxide composites as thermal energy storage materials

Mehrali, M. *et al. Energy*, 2013, 58, 628–634.

Palmitic acid/graphene oxide (PA/GO) as phase change materials (PCMs) prepared by vacuum impregnation method, have high thermal conductivity. The GO composite was used as supporting material to improve thermal conductivity and shape stabilization of composite PCM. Scanning electronic microscopy, Fourier transformation infrared spectroscopy (FT-IR) and X-ray diffractometry were applied to determine microstructure, chemical structure and crystalloid phase of palmitic acid/GO composites, respectively. Differential scanning calorimetry (DSC) testing was done to investigate thermal properties which include melting and solidifying temperatures and latent heat. FT-IR analysis represented that the composite instruction of porous PA and GO were physical. The temperatures of melting, freezing and latent heats of the composite measured through DSC analysis were 60.45, 60.05 °C, 101.23 and 101.49 kJ/kg, respectively. Thermal cycling test showed that the form-stable composite PCM has good thermal reliability and chemical stability. Thermal conductivity of the composite PCM was improved by more than three times from 0.21 to 1.02. As a result, due to their acceptable thermal properties, good thermal reliability, chemical stability and great thermal conductivities, the prepared form-stable composites can be considered as highly conductive PCMs for thermal energy storage applications.

14/02089 Progress in the development of solid–gas sorption refrigeration thermodynamic cycle driven by low-grade thermal energy

Li, T. X. *et al. Progress in Energy and Combustion Science*, 2014, 40, 1–58.

Heat-powered solid–gas sorption refrigeration technology has been regarded as one of the effective methods for reutilization of low-grade thermal energy such as industrial waste heat, renewable energy, and exhaust gases from engines. A number of advanced solid sorption refrigeration systems have been developed to improve energy efficiency by reducing the primary energy consumption as the recognition of energy saving. These advanced solid sorption refrigeration cycles mainly include heat recovery sorption cycle, mass recovery sorption cycle, mass and heat recovery sorption cycle, double/multi-effect sorption cycle, combined double-way sorption cycle, double-effect and double-way sorption cycle, two/multi-stage sorption cycle, etc. In this paper, the progress in the development of solid–gas sorption refrigeration thermodynamic cycle is reviewed. The operating principles of these advanced solid–gas sorption refrigeration cycles are introduced in detail, and the representative working performances of different sorption refrigeration cycles are presented and compared. Moreover, the key problems of advanced sorption refrigeration cycles are described and discussed. Finally, the future development of solid–gas sorption refrigeration cycle is also proposed.

14/02090 Regeneration performance of concentrated CO_2-rich alkanolamine solvents: the first step study of a novel concept for reducing regeneration heat consumption by using concentration swing absorption technology

Yan, S. *et al. Chemical Engineering and Processing: Process Intensification*, 2013, 70, 86–94.

A concept called 'concentration swing absorption' (CSA) is presented in order to save CO_2 regeneration heat requirements. In this process, the initial lean-CO_2 solvent is executed to form the so-called initial CO_2-rich solvent (ICRS) by absorbing CO_2, then ICRS is split into the concentrated CO_2-rich solvent (CCRS) phase and the diluted phase (mainly water). And only CCRS is regenerated in the stripper. Regeneration characteristics of CCRS were investigated as the first step study of CSA. Results showed that compared to the direct regeneration of ICRS, concentrating ICRS before regeneration cannot only improve the regeneration performance, but also reduce the regeneration temperature. Despite the increase of solvent viscosity hindering the CO_2 molecular diffusion of regeneration, ICRS should be concentrated to become the special CCRS with higher concentration beyond its unique critical concentration range. Moreover, based on the energy analysis of CSA considering the reboiler heat duty and energy required to concentrate ICRS by taking 30 wt% monoethanolamine as an example, theoretically the overall CO_2 regeneration heat requirement may be decreased considerably to 2739.98 kJ/kg of CO_2 by about 34.78% in the future when ICRS was concentrated to 60 wt%.

14/02091 SePTA – a new numerical tool for simultaneous targeting and design of heat exchanger networks

Wan Alwi, S. R. *et al. Computers & Chemical Engineering*, 2013, 57, 30–47.

Pinch analysis is an established insight-based methodology for design of energy-efficient processes. Composite curves (CCs) is a popular pinch analysis tool to target the minimum energy requirements. An alternative to the CCs is a numerical technique known as the problem table algorithm (PTA). PTA however, does not show individual hot and cold streams heat cascades and cannot be used for design of heat exchanger networks (HEN). This paper introduces the segregated problem table algorithm (SePTA) as a new numerical tool for simultaneous targeting and design of a HEN. SePTA shows profiles of heat cascade across temperature intervals for individual hot and cold streams, and can be used to simultaneously locate pinch points, calculate utility targets and perform SePTA heat allocation (SHA). The SHA can be represented on a new SePTA network diagram (SND) that graphically shows a heat exchanger network together with the amount of heat exchange on a temperature interval scale. This paper also shows that SePTA and SND can be a vital combination of numerical and graphical visualization tools for targeting and design of complex HENs involving stream splitting, threshold problems and multiple pinches.

14/02092 Simulation and experimental validation of soil cool storage with seasonal natural energy

Yang, T. *et al. Energy and Buildings*, 2013, 63, 98–107.

For the purpose of reducing energy consumption by summer air conditioning and utilizing renewable resources, this paper presents a new type of soil cool storage system with seasonal natural cold source In the cool storage system, the natural cool energy is stored in soil by ground heat exchanger during the cold season and is extracted for space cooling in the summer. Based on film moisture migration theory, a moisture-heat transfer coupling mathematical model is brought up to describe the charging and discharging processes of freeze–thaw phase change of the soil. Besides, a new method is presented that variable time step size is used to solve non-linear phase change problems numerically. Moreover, a comparison of the model predictions and experimental data shows that the model has good prediction accuracy. The parametric studies indicate that the soil cool storage system full meets the air conditioning needs and has excellence in economic performance. The research results prove that the feasibility of inter-seasonal cool storage system using shallow soil in severe cold regions.

14/02093 Study of the KNO_3–$LiNO_3$ and KNO_3–$NaNO_3$–$LiNO_3$ eutectics as phase change materials for thermal storage in a low-temperature solar power plant

Roget, F. *et al. Solar Energy*, 2013, 95, 155–169.

For heat storage applications, the solid–liquid phase changes of the $LiNO_3$–KNO_3 and $LiNO_3$–KNO_3–$NaNO_3$ mixtures of eutectic compositions have been investigated by differential scanning calorimetry and with a home built calorimeter working on large samples – typically 500 g. The design of the new calorimeter matches at best the geometry and the thermal transfers in the industrial application. The kinetics of crystallization has been particularly studied. Density measurements of the salts in the liquid state allowed to calculate the volumetric storage capacity.

14/02094 The effect of variable viscosity on the flow and heat transfer of a viscous Ag-water and Cu-water nanofluids

Vajravelu, K. *et al. Journal of Hydrodynamics, Ser. B*, 2013, 25, (1), 1–9.

A numerical study is carried out to study the effects of the temperature dependent viscosity on the flow and heat transfer of a nanofluid over a flat surface in the presence of viscous dissipation. The governing non-linear partial differential equations are transformed into non-linear ordinary differential equations, and are solved numerically by the Keller-box method. The numerical results indicate that the effect of nanoparticle volume fraction is to increase the heat transfer and hence enhance the thermal boundary layer thickness. This is true even in the presence of variable viscosity and the viscous dissipation. Furthermore, the results obtained for heat transfer characteristics with nanoparticles reveal many interesting behaviours that warrant further study on the effects of the 'nano-solid-particles'.

14/02095 Thermal conductivity of high porosity alumina refractory bricks made by a slurry gelation and foaming method

Shimizu, T. *et al. Journal of the European Ceramic Society*, 2013, 33, (15–16), 3429–3435.

Alumina has high heat resistance and corrosion resistance compared to other ceramics such as silica or mullite. However, for its application to refractory bricks, its high thermal conductivity must be reduced. To reduce this thermal conductivity by increasing the porosity, a gelation of slurry method that can produce high porosity solid foam was applied here to produce the alumina refractory brick. This method was successfully applied to produce alumina foam with high porosity and thermal conductivity of the foam is evaluated. At room temperature, the thermal conductivity was about 0.12 W/mK when the foam density was 0.1 g/cm^3. At elevated temperature above 783 K, thermal conductivity of the foam was strongly affected by heat radiation and increased with increasing temperature, in contrast to the thermal conductivity of alumina itself, which decreased with increasing temperature. The alumina foams developed here achieved sufficient thermal insulating properties for use in refractory bricks.

14/02096 Thermal energy storage and release of a new component with PCM for integration in floors for thermal management of buildings

Royon, L. *et al. Energy and Buildings*, 2013, 63, 29–35.

Lightweight envelopes (used primarily for economic reasons) are widely used in modern buildings but their low thermal capacity does not allow an optimal thermal comfort situation to be obtained in summer period. A solution is proposed here by using phase change materials (PCMs) incorporated in building structures to increase their thermal inertia without increasing their volume. A new polymer composite PCM containing 85% of paraffin, with a latent heat of melting of 110 kJ/kg and a melting point at about 27 °C, is incorporated in a hollow concrete floor panel. Experimental investigation on thermal behaviour is presented to study the response to a temperature variation. Results clearly show the influence of PCM, namely a decrease of the surface wall temperature amplitude and an increase of thermal energy stored. A numerical simulation with COMSOL Multiphysics® software confirms the enhancement of the floor inertia by the incorporation of the PCM. The simulation provides design guidelines for the thermal management system to minimize the quantity and size of PCM.

14/02097 Thermal energy storage strategies for effective closed greenhouse design

Vadiee, A. and Martin, V. *Applied Energy*, 2013, 109, 337–343.

The closed greenhouse is an innovative concept in sustainable energy management. In principle, it is designed to maximize the utilization of solar energy through the seasonal storage. In a fully closed greenhouse, there is not any ventilation window. Therefore, the excess sensible and latent heat must be removed, and can be stored using seasonal and/or daily thermal storage technology. This stored excess heat can then be utilized later in order to satisfy the thermal load of the greenhouse. Thermal energy storage (TES) system should be designed based on the heating and cooling load in each specific case. Underground thermal energy storage (UTES) is most commonly chosen as seasonal storage. In addition, a stratified chilled water (SCW) storage or a phase change material (PCM) storage could be utilized as short-term storage system in order to cover the daily demands and peak loads. In this paper, a qualitative economical assessment of the concept is presented. Here, a borehole thermal energy storage (BTES) system is considered as the seasonal storage, with a PCM or a SCW daily storage system to manage the peak load. A BTES primarily stores low temperature heat such that a heat pump would be needed to supply the heat at a suitable temperature. A theoretical model has been developed using TRNSYS to carry out the energy analysis. From the economic feasibility assessment, the results show that the concept has the potential of becoming cost effective. The major investment for the closed green-

house concept could be paid within 7–8 years with the savings in auxiliary fossil fuel considering the seasonal TES systems. However, the payback time may be reduced to 5 years if the base load is chosen as the design load instead of the peak load. In this case, a short-term TES needs to be added in order to cover the hourly peak loads.

14/02098 Thermo-dynamical process simulation of dilution refrigerator
Pradhan, J. *et al. Cryogenics*, 2013, 57, 158–165.
The design, analysis and optimization of a dilution refrigerator are carried via simulation of the thermo dynamical processes. To this end the authors have developed a comprehensive numerical simulation model, simulation of integrated dilution refrigerator for optimization (SIDFO) based on enthalpy–balance considerations taking into account for several important micro-effects which are normally ignored by existing methods. The simulation has produced several unique results of the underlying phenomena occurring at various stages of the very low temperature process presented in this paper. The corresponding simulation results are compared with published experimental data of operational machines and found to comply well. The presence of ^{4}He in the circulating gas and its consequences for the generalized cooling power is also thoroughly examined.

14/02099 Thermoeconomic design optimization of a thermo-electric energy storage system based on transcritical CO_2 cycles
Morandin, M. *et al. Energy*, 2013, 58, 571–587.
The conceptual design of a thermo-electric energy storage system for large-scale electricity storage is discussed in this work by showing the results of the thermoeconomic optimization of three different system configurations that were identified in previous works. The system is based on transcritical CO_2 cycles, water storage and salt-water ice storage and is designed for a capacity of 2 h discharge and equal charge and discharge power of 50 MW. A two-step optimization procedure is used. The system intensive design parameters are optimized at the master level through a genetic algorithm. The optimal cycle mass flow rates are calculated in a nested linear programming step where the heat integration between the cycles is optimized subject to the heat transfer feasibility imposed through pinch analysis cascade calculations. The synthesis of the heat exchanger network and of the storage tank systems was solved through a set of heuristic rules. Equipment purchasing costs were estimated by means of cost functions that were built on vendors' quotations. The results are discussed by showing the Pareto fronts of the three optimization cases and the trends of the decision variables along each optimal front. Nine solutions are discussed in more detail by showing the values of the design parameters and the process flow diagrams including storage and heat exchanger layouts. Design guidelines are then formulated which can be used in future works for detail plant design. The topological features that are found to maximize the system performance at the minimum costs are: superheating before the CO_2 heat pump, two independent systems of hot water storage tanks above and below the ambient temperature, and air cooling at the heat pump side. The design parameters that affect significantly the costs and performances are the cycle pressures. These are in fact directly associated with temperature differences both at the cold and hot storage sides which should be carefully optimized to obtain the best trade-off between exergy losses and costs for heat exchangers. Due to the change in specific heat of the supercritical CO_2 along the temperature range of hot water storage, a system of multiple storage tanks was used. Intermediate storage tanks help reduce significantly the temperature differences at the hot storage side and therefore their number represent another critical design parameter that must be optimized to achieve the best trade-off between costs and performances.

11 ENGINES

Power generation and propulsion, electrical vehicles

14/02100 Experimental investigations on high octane number gasoline formulations for internal combustion engines
Cerri, T. *et al. Fuel*, 2013, 111, 305–315.
The attempt to achieve higher and higher levels of specific power output and efficiency has increased the complexity of the design process of both the engine and its management system. Among the different issues, it is also necessary to take into account the chemical and physical characteristics of the available fuels. In order to study the behaviour of some gasoline formulations characterized by a high octane number, the authors have carried out an experimental activity to understand how each fuel sample could improve the performances of a modern naturally aspirated spark ignition (SI) engine for passenger cars. The new fuel formulations were characterized by different contents of olefins and oxygen, the latter through the presence of oxygenated compounds like ethyl tert-butyl ether or methyl tert-butyl ether. The experimental campaign consisted in measurements of the maximum brake torque curve up to knock onset and the corresponding knock intensity, at wide open throttle (WOT) and partial load operating conditions, for each tested gasoline sample. The results of the data analysis show that the evaluation of the enhanced characteristics of a gasoline cannot be done by considering only the increase of the knock limit. Although a gasoline is generally labelled only by its research octane number (RON), it can extend the benefits due to particular chemical formulation from full load up to part load conditions and, may be, in transient situations, as pointed out in this work. A naturally aspirated SI engine, under steady operation and fuelled by high octane number gasolines, cannot provide a higher power output at WOT condition only by modifying the spark timing, if this engine has already been correctly optimized by the manufacturer before introducing it on the market. As a result, to achieve higher levels of power output it is necessary to modify the compression ratio, the variable intake system and valve timing strategies and so on, in order to exploit the high octane number offered by the new gasolines tested. Moreover, the analysis of the experimental data has also confirmed that the RON index is less important than the motor octane number at high engine speeds and loads, useful to characterize the octane requirement for modern engines. Furthermore, a standard deviation analysis has been conducted on the burned mass fraction parameter to understand if the different characteristics of gasolines could give advantages in terms of reduction of the cyclic combustion variability. The results of the data analysis showed that the fuel formulations with higher content of oxygenated compounds exhibit a better behaviour, highlighting a smaller coefficient of variation especially when reducing the load. This aspect could be considered one of the possible reasons of an improvement of the vehicle drivability.

14/02101 Fuel flexible distributed combustion for efficient and clean gas turbine engines
Khalil, A. E. E. and Gupta, A. K. *Applied Energy*, 2013, 109, 267–274.
The need for fuel flexible ultra-low emission gas turbine combustors is imminent to secure future power needs. Distributed combustion technology is demonstrated to provide significant performance improvement of gas turbine combustors including uniform thermal field in the entire combustion chamber (improved pattern factor) at very high combustion intensity, ultra-low emission of NO_x and CO, low noise, enhanced stability, higher efficiency and alleviation of combustion instability. Distributed reaction conditions were achieved using swirl for desirable controlled mixing between the injected air, fuel and hot reactive gases from within the combustor prior to mixture ignition. In this paper, distributed combustion is further investigated using a variety of fuels. Gaseous (methane, diluted methane, hydrogen-enriched methane and propane) and liquid fuels, including both traditional (kerosene) and alternate fuels (ethanol) that cover a wide range of calorific values are investigated with emphasis on pollutants emission and combustor performance with each fuel. For liquid fuels, no atomization or spray device was used. Performance evaluation with the different fuels was established to outline the flexibility of the combustor using a wide range of fuels of different composition, phase and calorific value with specific focus on ultra-low pollutants emission. Results obtained on pollutants emission and OH* chemiluminescence for the specific fuels at various equivalence ratios are presented. Near distributed combustion conditions with less than 8 ppm of NO emission were demonstrated under novel premixed conditions for the various fuels tested at heat (energy) release intensity of 27 MW/m^3-atm. and a rather high equivalence ratio of 0.6. Higher equivalence ratios lacked favourable distributed combustion conditions. For the same conditions, CO emission varied for each fuel; less than 10 ppm were demonstrated for methane-based fuels, while heavier liquid fuels provided less than 40 ppm CO emissions. Lower emissions of NO (<4.5 ppm) were also demonstrated at lower equivalence ratios. This demonstration outlines the combustor ability for fuel flexibility without any modifications to the combustor injectors, while maintaining high performance. Further reduction of NO_x can be possible by establishing true distributed combustion condition, in particular at higher equivalence ratios.

14/02102 Ignition and kinetic modeling of methane and ethane fuel blends with oxygen: a design of experiments approach

Aul, C. J. *et al. Combustion and Flame*, 2013, 160, (7), 1153–1167.

A series of shock-tube experiments and chemical kinetics modelling calculations were performed to investigate the ignition behaviour of methane and ethane with oxygen in regions which are not presently well understood and in a much more comprehensive manner than what has been done previously. Test conditions were determined using a statistical design of experiments approach which allows the experimenter to probe a wide range of variable factors with a comparatively low number of experimental trials. A matrix of 22 mixtures was developed using this statistical approach for binary fuel blends of 100% methane to 100% ethane; pressure ranges of 1, 11–16 and 25–31 atm; equivalence ratios of 0.5, 1.0 and 2.0; over a temperature range of 1154–2248 K, and argon dilutions of 98%, 95%, 85% and 75%. Details on the relatively new high-pressure shock-tube facility are also provided. The experimental results were used to validate a detailed chemical kinetics model. The model considers hydrocarbons C_1–C_4 and has been developed in a hierarchical manner grounded with fundamental kinetics and experimentally validated by data from shock tubes and rapid compression machines, flow and jet-stirred reactors, and flame speed measurements. The important reactions are highlighted and the pertinent rate constants are described.

14/02103 Impact of alternative fuels on performance and pollutant emissions of a light duty engine tested under the new European driving cycle

Armas, O. *et al. Applied Energy*, 2013, 107, 183–190.

Two alternative fuels, a gas-to-liquid fuel from a low temperature Fischer–Tropsch process and a biodiesel produced from animal fats, have been tested using a light duty diesel engine with road load simulation under the New European Driving Cycle. The engine used has a variable geometry turbocharger, exhaust gas recirculation with cooling, common rail with split fuel injection and diesel oxidation catalyst. Regulated emissions have been evaluated and noticeable reductions in total hydrocarbon and carbon monoxide were observed with both alternative fuels whereas only slight decrease was obtained in NO_x emissions with biodiesel. With respect to results on particle matter, important reductions in both particle number and particle mass were obtained with both alternative fuels.

14/02104 Large-eddy simulations of turbulent flows in internal combustion engines

Banaeizadeh, A. *et al. International Journal of Heat and Mass Transfer*, 2013, 60, 781–796.

Large-eddy simulations (LES) of turbulent spray combustion in internal combustion engines are conducted with a new hybrid Eulerian–Lagrangian methodology. In this methodology, the Eulerian filtered compressible gas equations are solved in a generalized curvilinear coordinate system with high-order finite difference schemes for the turbulent velocity and pressure. However, turbulent mixing and combustion are simulated with the two-phase compressible scalar filtered mass density function (FMDF) and Lagrangian spray models. The LES/FMDF model is used for simulation of in-cylinder turbulent flow and spray mixing and combustion in three flow configurations: (1) a poppet valve in a sudden expansion, (2) a simple piston–cylinder assembly with a stationary valve and (3) a realistic single-cylinder, direct-injection spark–ignition (DISI) engine. The flow statistics predicted by the LES model are shown to compare well with the available experimental data for (1) and (2). The computed in-cylinder flow for the third configuration shows significant cycle-to-cycle variations. The flow in the DISI engine is also highly inhomogeneous and turbulent during the intake stroke, but becomes much more homogeneous and less turbulent in the compression stroke. Simulations of spray, mixing and combustion in the DISI engine indicate the applicability of the LES/FMDF model to internal combustion engines and other complex combustion systems.

14/02105 Simulation on the effect of the combustion parameters on the piston dynamics and engine performance using the Wiebe function in a free piston engine

Kim, J. *et al. Applied Energy*, 2013, 107, 446–455.

Numerical simulations were conducted to observe the relationship between the combustion phase and the piston dynamics in a free piston engine. The simulations were conducted with commercial software, MATLAB/SIMULINK®. The Wiebe function was used to simulate the combustion process. The combustion parameters such as combustion duration and the spark timing were varied at various piston initial velocities at compression stroke. The indicated mean effective pressure (IMEP) and the mass fraction burned (MFB) were analysed as indicators of the engine performance. Under given combustion duration conditions, the minimum ignition advance for best torque (MBT) timing was first retarded towards top dead centre (TDC) and consequently advanced away from TDC as the piston initial velocity increased. An MBT timing curve was plotted against various spark timings and piston initial velocities in a map. There existed a peak IMEP value along this MBT curve. Longer combustion duration brought negative effects on the IMEP due to larger deviation from the quasi-constant volume combustion, thus lowering the efficiency. The velocity profile of the piston was plotted against the displacement with a contour of every 10% increment of mass fraction burned in order to provide a clear visualization of the combustion process. The spark timing had to be advanced with high piston initial velocity or a long combustion duration condition in order to complete the combustion process near TDC. Mass fraction burned values at TDC showed a linear relationship with piston initial velocity values. This provided a general idea of how to vary the spark timing under a given piston initial velocity condition to achieve the best conversion efficiency from combustion to work regardless of the combustion duration.

14/02106 The challenges and strategies of butanol application in conventional engines: the sensitivity study of ignition and valve timing

Deng, B. *et al. Applied Energy*, 2013, 108, 248–260.

The study approach of this paper is to combine experiment and simulation on using butanol as fuel in gasoline engine. First, experiments were performed under full load on a single cylinder spark ignition engine fuelled with 35%vol butanol–gasoline blend and the pure gasoline, respectively. The performance and operating parameters were measured. The experimental results showed that with the butanol addition, the ignition timing could be advanced without obvious knocking for higher combustion efficiency. The engine presented superior performance in power, fuel consumption, HC and CO emissions, but deteriorated the NO_x emissions largely. Then, a GT-Power simulation model was set-up and calibrated by experimental data. Therefore, the simulation model could be used to study the valve timing impact on engine performance. The simulation results indicated that the enlargement of overlap presented a good 'trade-off' effect, such as, decreased emissions (especially for NO_x), without deteriorating the torque and fuel consumption too much (except for extremity speeds of 3000 and 8500 rpm, which are not frequently-used in real road driving). The results also indicated that the HC and CO emissions depend more on the fuel properties, the power and NO_x emissions depend more on the operating parameters, and the fuel consumption is in between.

14/02107 The potential of using cocoa pod husks as green solid base catalysts for the transesterification of soybean oil into biodiesel: effects of biodiesel on engine performance

Ofori-Boateng, C. and Lee, K. T. *Chemical Engineering Journal*, 2013, 220, 395–401.

In this study, the feasibility of using potash from cocoa pod husks (CPHs) in the transesterification of soybean oil into biodiesel was investigated. Both supported (CPH/MgO) and unsupported (CPH ash) catalysts of potash prepared from CPH were used as green heterogeneous catalysts for biodiesel production. Under optimum conditions for the CPH/MgO-catalysed (oil-to-methanol ratio of 1 : 6, 60 °C, 60 min, 1 wt% of MgO-doped CPH ash catalyst) and the CPH-catalysed (60 °C, oil-to-methanol ratio of 1 : 6, 120 min, 1 wt% of CPH ash) transesterification reactions, biodiesel samples (98.7% and 91.4% yields for CPH/MgO and CPH ash catalysts, respectively) with specifications falling within the limits of the European biodiesel quality standard (EN 14112) were obtained. Brake thermal efficiencies and torque were measured for each fuel sample at different loads. Engine test showed a better performance for all the fuel samples (B100 and B40) with B40 showing close characteristics of petroleum diesel. Thus, this first report on the utilization of CPH as catalyst for biodiesel shows a high feasibility of producing green heterogeneous base catalysts commercially from CPH for sustainable biodiesel production.

Hybrid engine systems

14/02108 Environmental assessment of plug-in hybrid electric vehicles using naturalistic drive cycles and vehicle travel patterns: a Michigan case study

Marshall, B. M. *et al. Energy Policy*, 2013, 58, 358–370.

Plug-in hybrid electric vehicles (PHEVs) use grid electricity as well as on-board gasoline for motive force. These multiple energy sources make prediction of PHEV energy consumption challenging and also complicate evaluation of their environmental impacts. This paper introduces a novel PHEV energy consumption modelling approach and compares it to a second approach from the literature, each using actual trip patterns from the 2009 National Household Travel Survey. The first approach applies distance-dependent fuel efficiency and on-road electricity consumption rates based on naturalistic or real world,

driving information to determine gasoline and electricity consumption. The second uses consumption rates derived in accordance with government certification testing. Both approaches are applied in the context of a location-specific case study that focuses on the state of Michigan, USA. The two PHEV models show agreement in electricity demand due to vehicle charging, gasoline consumption, and life cycle environmental impacts for this case study. The naturalistic drive cycle approach is explored as a means of extending location-specific driving data to supplement existing PHEV impact assessments methods.

14/02109 Experimental investigation of the effects of diesel injection strategy on gasoline/diesel dual-fuel combustion

Ma, S. *et al. Applied Energy*, 2013, 109, 202–212.

This study investigates the effects of diesel injection strategies on combustion, emissions, fuel economy and the operation range with high efficiency and low emissions fuelled with gasoline/diesel dual fuel on a modified single-cylinder diesel engine. This gasoline/diesel dual-fuel combustion mode proposes port fuel injection of gasoline and direct injection of diesel fuel with rapid in-cylinder fuel blending. Single and double injection strategies were employed in the engine experiments at 1500 rev/min and 50 mg/cycle total equivalent diesel fuelling rate. The experimental results showed that this combustion mode had the capability of achieving high efficiency with near-zero NO_x and soot emissions by using an early injection timing of single (E-single) strategy with high gasoline ratio. Parameters were optimized in double injection strategy included the first and second injection timing, injected diesel mass split between the two injections and the premixed gasoline ratio. Based on the optimized results, the comparison between single and double injection strategies was investigated. Compared to other three injection strategies, the early second injection timing (E-SOI2) strategy achieved the lowest indicated specific fuel consumption (ISFC) of 173 g/kW h, the NO_x and soot emissions were below 0.2, 0.003 g/kW h respectively, but the maximum pressure rise rate (MPRR) was penalized, while the late second injection timing (L-SOI2) strategy was most favourable at reducing MPRR because of prolonged combustion duration. E-single and E-SOI2 strategies were difficult at high loads due to the high MPRR. Therefore, L-SOI2 strategy is an effective approach to expand the operation range to higher load. However, the upper load was limited by high soot emissions, which demanded increasing the diesel injection pressure. Under the operating conditions with optimized parameters, the maximum indicated mean effective pressure can be expanded up to 1.391 MPa by using L-SOI2 strategy with increased fuel mass while still maintaining good emissions and MPRR within a given criteria.

14/02110 Geodemographic analysis and estimation of early plug-in hybrid electric vehicle adoption

Saarenpää, J. *et al. Applied Energy*, 2013, 107, 456–464.

Electric vehicles and hybrids are expected to become increasingly common in the coming years. The implications of growing adoption depend on its geographical extent. For instance, vehicles that are chargeable from the electrical grid, such as plug-in hybrids, can introduce problems for the distribution network especially if the vehicle adoption is spatially concentrated. In this paper, the adoption of hybrid electric vehicles is analysed in heterogeneous areas. The main purpose is to study the interrelationships between early hybrid electric vehicle adoption and different demographic and socio-economic characteristics of the areas. It is further discussed how the results can be applied to estimate the upcoming plug-in hybrid adoption. As there is a vast amount of information in the various registers of the society, slowly being opened for free usage but not fully utilized so far, it is also of interest to study and demonstrate the usability of public register data in this context. This analysis suggests that certain characteristics of the areas strongly correlate with the hybrid electric vehicle adoption. The results of this study could be relevant, e.g. for electric distribution network planning, targeting policies to support cleaner vehicle adoption, marketing hybrid vehicles and locating charging stations.

14/02111 HC and CO emissions reduction by early injection strategy in a bioethanol blended diesel-fueled engine with a narrow angle injection system

Park, S. H. *et al. Applied Energy*, 2013, 107, 81–88.

The main purpose of this study was to investigate how a narrow angle injector affects the combustion and exhaust emissions characteristics in a single-cylinder diesel engine fuelled by diesel–bioethanol blends. This study focused on reducing HC and CO emissions in the exhaust emissions by the bioethanol blending of diesel. A narrow angle injector with an injection angle of 70° was used and compared with a conventional angle injector having a 156° injection angle. The bioethanol was blended with the conventional diesel up to 30% with 5% biodiesel. Experiments revealed that, in a narrow angle injector, the premixed combustion duration increased with bioethanol contents unlike the similar value of conventional injector. The premixed combustion phasing decreased with the increase of bioethanol in both injectors. The variation in the peak combustion pressure of the narrow angle injector was smaller than that of a conventional injector. In addition, the narrow angle injector induced a higher indicated mean effective pressure and a shorter ignition delay compared to the conventional injector. In terms of exhaust emissions characteristics, the low and stable ISHC and ISCO emissions can be achieved through the application of narrow angle injector to the diesel–bioethanol blends combustion. By the early injection combustion strategy, ISHC and ISCO emissions are significantly reduced.

Transport battery development

14/02112 Affordability of electric vehicles for a sustainable transport system: an economic and environmental analysis

Tseng, H.-K. *et al. Energy Policy*, 2013, 61, 441–447.

This paper compares the economic and environmental benefits of electric and hybrid electric vehicles with that of conventional vehicles. Without tax credits, only the hybrids without plug-in incur lifetime total costs equivalent to a conventional vehicle whereas the consumer affordability for all other vehicles is less encouraging and depends on changes in gasoline prices. With the provision of federal tax incentives, the lifetime total cost for all electric vehicle types that are driven for 120,000 miles over 12 years was found to be generally affordable with no more than 5% higher in lifetime total cost than a conventional vehicle, except the hybrid electric plug-in equipped with a 35-mile electric driving range. Results of sensitivity analysis reveal that a greater lifetime driven mileage would promote further overall cost savings even at a greenhouse gas abatement cost as low as $42/ton. The study has demonstrated the importance of an energy policy that includes tax credits to address the inadequacy of cost differentials and consumer affordability. The environmental benefits provided by the electric and hybrid electric vehicles should satisfy consumers' interest in protecting the environment, reducing the dependence on imported fossil fuels, and switching from traditional to alternative fuel vehicles.

14/02113 Copper vanadate as promising high voltage cathodes for Li thermal batteries

Hillel, T. and Ein-Eli, Y. *Journal of Power Sources*, 2013, 229, 112–116.

In this work a series of the $CuO–V_2O_5$ oxides, such as CuV_2O_6, $Cu_2V_2O_7$ and $Cu_5V_2O_{10}$, have been synthesized and evaluated as possible candidate cathode materials in high-voltage Li thermal batteries. The structure and morphology have been determined and the electrochemical properties at room temperature and elevated temperatures (525 °C) against Li metal alloy have been investigated. At room temperature, an increase in copper content in the vanadate has been found to provoke a gradual negative shift of the operating voltage plateau vs Li metal. Room temperature discharge capacity in a Li cell is relatively high and can exceed 350 $mAhgr^{-1}$. In a thermal Li cell configuration and at an elevated temperature a voltage plateau of 3.4 V at a current load of 100 $mA\,g^{-1}$ was achieved and a voltage plateau of 2.5 V was recorded with a current load of as high as 310 $mA\,g^{-1}$. Thus, copper-vanadate materials may be regarded as promising short-time–high-voltage cathodes for thermal Li batteries.

14/02114 Going electric: expert survey on the future of battery technologies for electric vehicles

Catenacci, M. *et al. Energy Policy*, 2013, 61, 403–413.

The paper describes the results of a survey carried out with leading European Union (EU) experts on the future costs of batteries for electric vehicles (EVs) and plug-in hybrid vehicles and the uncertainty surrounding them. Battery costs are one of the main components in the overall costs of EVs and improvements could be brought about by increased investments in research, development and demonstration (RD&D). Experts' judgements are collected to shed light on the inherently uncertain relationship between RD&D efforts and the consequent technical progress in batteries. The analysis of the experts' data results in a number of important policy recommendations to guide future RD&D choices and target commitments both for the EU and its member states.

14/02115 Influence of driving patterns on life cycle cost and emissions of hybrid and plug-in electric vehicle powertrains

Karabasoglu, O. and Michalek, J. *Energy Policy*, 2013, 60, 445–461.

This study compares the potential of hybrid, extended-range plug-in hybrid, and battery electric vehicles to reduce lifetime cost and life cycle greenhouse gas emissions under various scenarios and simulated driving conditions. The authors find that driving conditions affect economic and environmental benefits of electrified vehicles substantially: under the urban NYC driving cycle, hybrid and plug-in vehicles can cut life cycle emissions by 60% and reduce costs up to 20% relative to conventional vehicles. In contrast, under highway test conditions

(HWFET) electrified vehicles offer marginal emissions reductions at higher costs. NYC conditions with frequent stops triple life cycle emissions and increase costs of conventional vehicles by 30%, while aggressive driving (US06) reduces the all-electric range of plug-in vehicles by up to 45% compared to milder test cycles (like HWFET). Vehicle window stickers, fuel economy standards, and life cycle studies using average lab-test vehicle efficiency estimates are therefore incomplete: (1) driver heterogeneity matters, and efforts to encourage adoption of hybrid and plug-in vehicles will have greater impact if targeted to urban drivers vs highway drivers; and (2) electrified vehicles perform better on some drive cycles than others, so non-representative tests can bias consumer perception and regulation of alternative technologies. The authors discuss policy implications.

14/02116 Model-based state of charge and peak power capability joint estimation of lithium-ion battery in plug-in hybrid electric vehicles
Xiong, R. *et al. Journal of Power Sources*, 2013, 229, 159–169.
This paper uses an adaptive extended Kalman filter (AEKF)-based method to jointly estimate the state of charge (SoC) and peak power capability of a lithium-ion battery in plug-in hybrid electric vehicles (PHEVs). First, to strengthen the links of the model's performance with battery's SoC, a dynamic electrochemical polarization battery model is employed for the state estimations. To get accurate parameters, four different charge–discharge current were used to improve the hybrid power pulse characteristic test. Second, the AEKF-based method was employed to achieve a robust SoC estimation. Third, due to the PHEVs require continuous peak power for acceleration, regenerative braking and gradient climbing, the continuous peak power capability estimation approach was proposed. And to improve its applicability, a general framework for six-step joint estimation approach for SoC and peak power capability was proposed. Lastly, a dynamic cycle test based on the urban dynamometer driving schedule was performed to evaluate the real-time performance and robustness of the joint estimation approach. The results show that the proposed approach can not only achieve an accurate SoC estimate and its estimation error is below 0.02 especially with big initial SoC error; but also gives reliable and robust peak power capability estimate.

14/02117 Optimal recharging strategy for battery-switch stations for electric vehicles in France
Armstrong, M. *et al. Energy Policy*, 2013, 60, 569–582.
Most papers that study the recharging of electric vehicles (EVs) focus on charging the batteries at home and at the workplace. The alternative is for owners to exchange the battery at a specially equipped battery switch station (BSS). This paper studies strategies for the BSS to buy and sell the electricity through the day-ahead market. The authors determine what the optimal strategies would have been for a large fleet of EVs in 2010 and 2011, for the vehicle-to-grid (V2G) and the grid-to-vehicle (G2V) cases. These give the amount that the BSS should offer to buy or sell each hour of the day. Given the size of the fleet, the quantities of electricity bought and sold will displace the market equilibrium. Using the aggregate offers to buy and the bids to sell on the day-ahead market, the new prices and volumes transacted can be computed. While buying electricity for the G2V case incurs a cost, it would have been possible to generate revenue in the V2G case, if the arrivals of the EVs had been evenly spaced during the day. Finally, the authors compare the total cost of implementing the strategies with the cost of buying the same quantity of electricity from EDF.

14/02118 Preparation and characterization of size-uniform $Li[Li_{0.131}Ni_{0.304}Mn_{0.565}]O_2$ particles as cathode materials for high energy lithium ion battery
Xiang, X. *et al. Journal of Power Sources*, 2013, 230, 89–95.
Lithium-rich layered oxide, $Li[Li_{0.131}Ni_{0.304}Mn_{0.565}]O_2$ with uniform particle size, is prepared through co-precipitation of metal hydroxide with synergistic dispersion of polyvinylpyrrolidone and ethylene glycol and subsequent solid reaction with lithium hydroxide. The crystal structure and morphology of the prepared sample is characterized with X-ray diffraction and scanning electron microscope. It is found that the prepared sample is a solid solution of Li_2MnO_3 and $LiNi_{0.5}Mn_{0.5}O_2$, with uniform particle size of about 230 nm. Charge/discharge tests indicate that the prepared sample exhibits improved elevated-temperature discharge capacity and cycling stability. In the region of 3.0–4.8 V, the prepared sample delivers initially a 0.1 C (1 C = 263 mAh g^{-1}) capacity of 256 mAh g^{-1} at 50 °C and 205 mAh g^{-1} at 25 °C, and the 0.1 C capacity at 25 °C retains 178 mAh g^{-1} after 60 cycles. The capacity decay mechanism is understood in detail through dQ/dV analyses.

14/02119 Slot-die processing of lithium-ion battery electrodes – coating window characterization
Schmitt, M. *et al. Chemical Engineering and Processing: Process Intensification*, 2013, 68, 32–37.
Slot-die coating is actually the most used coating method for the manufacturing of lithium-ion battery electrodes. An easy way of reducing production costs is to increase the line capacity. Thus, the relatively high-viscous slurries are coated at continuously increasing velocities. Facing these higher and higher velocities, the main processing challenge is to ensure that the surface quality stays constant. Therefore this study investigated the coating of high-viscous anode slurries consisting of large graphite particles. Systematically detected conditions for which coating defects occurred were discussed and compared with different theoretical limits for stable coating conditions. Thereby the uniformity of the stable wet film was analysed and logged with a two-dimensional laser sensor system. Even though the detected break-up lines are, in some regions, congruent with the applied visco-capillary models, the appearing coating defects are not as expected in the literature. Furthermore, large particles and agglomerations may provoke an additional film break-up at small film thicknesses regardless of the coating speed. For stable conditions the roughness of the film increases when the dimensionless gap width increases.

14/02120 The effects of FEC (fluoroethylene carbonate) electrolyte additive on the lithium storage properties of NiO (nickel oxide) nanocuboids
Seng, K. H. *et al. Energy*, 2013, 58, 707–713.
Nanocuboid-shaped nickel oxide (NiO) has been synthesized using an optical floating zone furnace. It was found that the nanocuboids exhibit single crystalline nature, and have clean and sharp edges. Furthermore, the NiO nanocuboids were tested for their electrochemical performances as anode material for lithium-ion batteries in a coin-type half-cell. The effects of fluoroethylene carbonate (FEC) additive on the lithium storage performance were also investigated, which is the first of such studies for transition metal oxides. It was found that FEC has a positive effect on the cycling stability and also improves the rate performances of the nanocuboids. The capacity recorded at 0.1 C (100 mA g^{-1}) after 50 charge/discharge cycles is 1400 mAh g^{-1}. Lastly, the NiO nanocuboids can achieve very high rate capability of 12 C (12 A g^{-1}) with capacity of 312 mAh g^{-1}.

12 REFRACTORIES/ CERAMICS

Properties, production, applications

14/02121 A building integrated solar collector: all-ceramic solar collector
Yang, Y. *et al. Energy and Buildings*, 2013, 62, 15–17.
A type of all-ceramic flat plate solar collector is introduced. These all-ceramic solar collectors are made from ordinary ceramic and V–Ti black ceramic. The solar absorptance of black ceramic coatings is in the range of 0.93–0.97. The all-ceramic solar collector is characterized by low cost, long lifetime, no attenuation of absorptance, and building integration. The word 'integration' means not only that the solar elements are used as architectural elements in attractive, visible (or invisible), and not too costly ways, but also that the solar collectors should have the same lifetime with the building. They should replace other building elements or share roof materials with building roof. For example, they can act as balcony railings, or share the insulation layer. When the solar thermal collectors act as balcony railings, the thermal efficiency is about 471%. When solar collectors integrate with pitched building roofs, the thermal efficiency of all-ceramic solar system is more than 50%.

14/02122 A double-pane window with enclosed horizontal slats for daylighting in buildings in the tropics
Chaiwiwatworakul, P. and Chirarattananon, S. *Energy and Buildings*, 2013, 62, 27–36.
In the tropics, daylighting from a side window requires shading to intercept direct sunlight from the window while allowing penetration of daylight from sky. In this paper, daylighting from a double-pane glazed window with enclosed horizontal slats (slat window) was investigated for which it is situated on either north or south wall of a room. Full-scale experiments and simulations were conducted to characterize distribution of the interior daylight from the slat window under a real tropical climate. Performance of the slat window was evaluated in terms of the 'useful daylight illuminance', interior daylight availability and light power density (LPD) of an integrated dimmable lighting system. Empirical formulas were developed for determining annual

average LPD values of the dimmable lighting system over its served area. The LPD value can be used with a reduced form of the energy equation of Thailand's building energy code to evaluate the reduced annual electrical energy consumption for accreditation of the daylight use in a building. The analysis of life cycle cost proved that the daylighting from the slat window integrated with the dimmable lighting system is cost effective.

14/02123 A novel route to prepare weather resistant, durable antireflective films for solar glass

Xin, C. *et al. Solar Energy*, 2013, 93, 121–126.

Silica antireflective coatings by the base catalysed sol–gel process show poor mechanical property. In this study, the base-catalysed sol was modified by acid-catalysed polysiloxane and nano-TiO_2 sol. The single-layer antireflective films were prepared using spray-coating technology, the effects of transmission speed on the optical performance of the films were studied. The results show that the films derived from the modified sol have an excellent weather resistance. Its degradation of transmittance after damp-heat test is only 0.23%. The maximum transmittance of the antireflective solar glass with single layer coating is about 95.02% at 565 nm wavelength, which is about 3.36% higher than the substrate glass. The adhesion of the film is 5B and the pencil hardness is equal or higher than 3H. High transmittance, good mechanical properties and excellent durability make the films be suited to solar glass.

14/02124 Ceramic hollow fiber membrane distributor for heterogeneous catalysis: effects of membrane structure and operating conditions

Meng, L. *et al. Chemical Engineering Journal*, 2013, 223, 356–363.

A ceramic hollow fibre membrane distributor was proposed for the micro-scale distribution of reactants in heterogeneous catalytic reaction. To evaluate the feasibility and the performance of the ceramic hollow fibre membrane-based reactant distribution, phenol hydroxylation with hydrogen peroxide (H_2O_2) over TS-1 solid catalysts was selected as a model reaction. The effects of membrane structural parameters of ceramic hollow fibre membrane on the micro-scale distribution and the reaction selectivity were studied in detail. The influence of operation conditions such as hydrogen peroxide flow rate, stirring rate and phenol/H_2O_2 molar ratio on the membrane distribution process was discussed. The ceramic hollow fibre membrane with small pore size and proper gradient in the pore structure was demonstrated to have a promotion effect on the reaction selectivity, which indicated its ability to generate uniform droplets in micro-scale. In addition, the increase of H_2O_2 flow rate and/or stirring rate can result in an improvement of reaction selectivity. Because of its controllable structure, high chemical stability and high packing density, the ceramic hollow fibre membrane distributor has potential for widespread applications in heterogenous catalysis.

14/02125 Comparison of approaches to minimize fouling of a UF ceramic membrane in filtration of seawater

Xu, J. *et al. Chemical Engineering Journal*, 2013, 223, 722–728.

In this study, several anti-fouling approaches including coagulation conditions ($FeCl_3$ dosage and feed pH), air-enhanced backwash (AEB) conditions (backwash interval and AEB duration) and chemical cleaning conditions (reagents, soak time and temperature) were evaluated to enhance the feasibility of a commercial ultrafiltration (UF) membrane as a pretreatment of reverse osmosis (RO) seawater desalination. A tubular commercial ceramic UF membrane with a surface layer of zirconium dioxide (ZrO_2) and a supporting layer of α-alumina oxide (α-Al_2O_3) was employed in this study. The results showed that ferric coagulation was functional to enhance the performance of ceramic UF for seawater treatment, especially on chemical oxygen demand removal. The trial of cleaning demonstrated that the performance of NaClO was much better than that of HNO_3 under various evaluated pH values. The relevant additional experiments showed that the cleaning efficiency increased with NaClO concentration, soak time and soak temperature but decreases when soak temperature was up to 60 °C. An important finding of this study is that the fouled membrane from coagulation-filtration trial can be easily and quickly recovered by acid cleaning regents followed by NaClO solution. Furthermore, short backwash interval performed more efficiently. However, it is certain that both backwash interval and AEB duration enhanced less than other approaches on the permeate quality. This study finally summarized the operating condition of each anti-fouling approach for the further potential application of UF ceramic membrane as a pretreatment of RO seawater desalination.

14/02126 Dry gas–solid carbonation in fluidized beds of $Ca(OH)_2$ and nanosilica/$Ca(OH)_2$ at ambient temperature and low CO_2 pressure

Pontiga, F. *et al. Chemical Engineering Journal*, 2013, 222, 546–552.

This work presents a study on the chemisorption of CO_2 by a bed of $Ca(OH)_2$ powder subjected to the flow of a dry CO_2/N_2 gas mixture (1 vol.% CO_2) at ambient temperature and atmospheric pressure. The amount of CO_2 and vapour water in the effluent gas from the fluidized bed is analysed by means of Fourier transform infrared spectrophotometry. The results obtained indicate that, even in an almost dry atmosphere ($RH \leq 0.01\%$), CO_2 capture in the fluidized bed occurs by chemisorption on $Ca(OH)_2$, as inferred from the rise of vapour water at the end of the fast carbonation phase. The use of nanosilica as an additive increases the gas–solids contact efficiency and, therefore, enhances CO_2 chemisorption on $Ca(OH)_2$ particles. This process is initially activated by free molecular water physisorbed on the material and becomes autocatalysed by water produced from $Ca(OH)_2$ carbonation. Accordingly, the addition of hydrophilic nanosilica, capable of retaining higher amounts of free molecular water, yields a further enhancement of the CO_2 fast sorption capacity.

14/02127 Energy and exergy analysis of the silicon production process

Takla, M. *et al. Energy*, 2013, 58, 138–146.

This study used energy and exergy analysis to evaluate two industrial and one ideal (theoretical) production process for silicon. The industrial processes were considered in the absence and presence of power production from waste heat in the off-gas. The theoretical process, with pure reactants and no side-reactions, was used to provide a more realistic upper limit of performance for the others. The energy analysis documented the large thermal energy source in the off-gas system, while the exergy analysis documented the potential for efficiency improvement. The authors found an exergetic efficiency equal to 0.33 ± 0.02 for the process without power production. The value increased to 0.41 ± 0.03 when waste heat was utilized. For the ideal process, an exergetic efficiency of 0.51 was found. Utilization of thermal exergy in an off-gas of 800 °C increased this exergetic efficiency to 0.71. Exergy destructed due to combustion of by-product gases and exergy lost with the furnace off-gas were the largest contributors to the thermodynamic inefficiency of all processes.

14/02128 Enhanced effect of carbon nanotube on mechanical and electrical properties of cement composites by incorporation of silica fume

Kim, H. K. *et al. Composite Structures*, 2013, 107, 60–69.

Utilization of silica fume in carbon nanotube (CNT)/cement composites was recently proposed as a mean of improving the dispersion of CNTs and enhancing the interfacial interaction between CNTs and the hydration products. The present study focuses on the enhanced effect of CNTs on mechanical and electrical properties of cement composites by incorporation of silica fume. A qualitative analysis using scanning electron microscopy images was carried out to observe the surface morphology and microstructure of cement composites with different amounts of silica fume and CNT addition. The effects of silica fume addition on the porosity, compressive strength, and electrical resistance of the CNT/cement composites were then systematically investigated. It was found that the improved dispersion of CNTs by incorporation of silica fume might yield the enhancement of the mechanical and electrical properties of CNT/cement composites, whereas the CNT additions in cement composite without silica fume had an insignificant effect on the mechanical and electrical properties of the cement composites.

14/02129 Experimental investigation of mass transfer of active ions in silica nanofluids

Keshishian, N. *et al. International Communications in Heat and Mass Transfer*, 2013, 46, 148–153.

In this paper the effect of silica nanoparticles on mass transfer was studied in circular tube by using electrochemical limiting current technique in both laminar and turbulent flow regimes. Underdeveloped concentration and fully developed hydrodynamic profile was considered. Silica nanoparticles with the size range of 7–13 nm was used to prepare electrolyte nanofluid. Base fluid was composed of equimolar potassium ferri-ferrocyanide and sodium hydroxide. Measurements for laminar regime indicated that mass transfer coefficient increased with nanofluid volume fraction up to 0.0057% and decreased with increasing the volume fraction of nanoparticles further. Maximum enhancement in mass transfer reached 21% at Reynolds number of 326. In turbulent flow regime no enhancement was recognized due to the addition of silica nanoparticles to the base electrolyte solution.

14/02130 Fused calcium zirconate for refractory applications

Schafföner, S. *et al. Journal of the European Ceramic Society*, 2013, 33, (15–16), 3411–3418.

This paper investigates dense $CaZrO_3$ produced by electric arc melting and compares it to solid state synthesized $CaZrO_3$. The fused $CaZrO_3$ had a considerable lower porosity than the solid state synthesized material, however due to evaporation of some CaO during the electric

arc melting the stoichiometric ratio of CaO/ZrO_2 was slightly smaller than one, resulting in the formation of cubic ZrO_2 as a second phase. To determine the local phase distribution the materials were investigated with electron backscatter diffraction (EBSD) in addition to integral X-ray diffraction. The vibration polishing of the ceramics resulted in excellent EBSD patterns. Die pressed cylinders of the fused material led to a porosity as low as 14.3%. The linear thermal expansion coefficient from 25 to 1000 °C was $10.45 \times 10^{-6} K^{-1}$. The cold isostatic pressing of larger crucibles resulted in higher porosity of 15.9–16.5%. The EBSD analysis and the cold isostatic pressed crucibles can be applied in corrosion tests for titanium melts.

14/02131 Galvanic corrosion of Mg–Zr fuel cladding and steel immobilized in Portland cement and geopolymer at early ages

Rooses, A. *et al. Journal of Nuclear Materials*, 2013, 435, (1–3), 137–140.

Galvanic corrosion behaviour of Mg–Zr alloy fuel cladding and steel has been studied in ordinary Portland cement and Na–geopolymer. Portland cements implied the worse magnesium corrosion performances due to the negative effects of cement hydrates, grinding agents and gypsum on the galvanic corrosion. Galvanic corrosion in Na–geopolymer paste remains very low. Silicates and fluoride from the geopolymer activation solution significantly improve the corrosion resistance of the magnesium alloy while coupling with a cathode.

14/02132 Hybrid laminated-glass plate: design and assessment

Foraboschi, P. *Composite Structures*, 2013, 106, 250–263.

This paper is focused on laminated glass plate designed with the 'sacrificial ply' concept: the glass layer that collects the live loads is considered as broken (i.e. it is not considered), independently of whether or not it is fractured. Accordingly, the load-bearing system is composed of: heat-strengthened (or annealed) glass layer, plus interlayer, plus toughened (tempered or chemically strengthened) glass layer. Hence, the laminated glass plate is a hybrid. The first part of the paper derives the constitutive law of the interlayer materials that belong to the latest generation. Then, the behaviour of the laminated glass plate is predicted by using this new constitutive law in lieu of the constitutive law of traditional interlayer materials, and the results are analysed. The second part discusses the results of a theoretical analysis conducted on products available on the architectural marketplace that encompass glass structural applications. These results prove that the ultimate load is dictated by the toughened glass only if the stiffness of the interlayer surpasses a critical value; otherwise, it is dictated by the less resistant glass. However, the critical value is very high. Moreover, the results prove that assessment cannot use practical or simplified expressions (e.g. effective thickness), since these expressions provide the maximum stress in the plate but not in each layer.

14/02133 Manufacture of calcium-based sorbents for high temperature cyclic CO_2 capture via a sol–gel process

Luo, C. *et al. International Journal of Greenhouse Gas Control*, 2013, 12, 193–199.

A CaO sorbent with high reactivity for cyclic high-temperature CO_2 capture was synthesized using a standard sol–gel process with citric acid as the chelation agent. The cyclic CO_2 capture performance of the new sorbent was compared with that of the sorbents derived from commercial micro- and nano-sized $CaCO_3$. The new CaO sorbent achieved a high CO_2 capture capacity of 0.51 g CO_2/g sorbent under mild calcination conditions and retained an acceptable CO_2 capture capacity of 0.20 g CO_2/g sorbent under severe calcination conditions after 20 cycles, much higher than those of the sorbents derived from commercial $CaCO_3$ under the same reaction conditions. In addition, the new sorbent had a very rapid reaction rate at the initial reaction stage, achieving a calcium conversion ratio of 60% within 20 s. Microscopic images showed that well-dispersed particles with an average size of about 200 nm were formed within the sorbent. The new sorbent also had a better sintering-resistant property than the other sorbents tested during multiple calcination/carbonation cycles.

14/02134 Monitoring the performance of single and triple junction amorphous silicon modules in two building integrated photovoltaic (BIPV) installations

Eke, R. and Senturk, A. *Applied Energy*, 2013, 109, 154–162.

Mugla is located in south-west Turkey at 37°13′N latitude and 28°36′E longitude with yearly sum of horizontal global irradiation exceeding 1700 kW h/m^2. Mugla has a Mediterranean climate characterized by long, hot and dry summers with cool and wet winters. Mugla Sitki Kocman University is the largest photovoltaic (PV) park in Turkey consisting of 100 kWp installed PV power systems (PVPSs) with different PV applications. The 40 kWp building-integrated photovoltaic (BIPV) system which is the first and largest in Turkey was installed on the façade and the two towers of the staff block of the Mugla Sitki Kocman University in February 2008. Triple junction amorphous silicon PV modules are used on the façade and single junction amorphous silicon PV modules are used on the east and west towers of the building. In this paper, the 40 kWp BIPV system in Mugla, Turkey is presented, and its performance is evaluated. Energy rating (kW h/kWp energy yield), efficiencies and performance ratios of both applications are also evaluated for 36 months of operation. Daily, monthly and seasonal variations in performance parameters of the BIPV system in relation to solar data and meteorological parameters and outdoor performance of two reference modules (representing the modules on façade and towers) in a summer and a winter day are also investigated.

14/02135 Performance of a daylight-redirecting glass-shading system

Appelfeld, D. and Svendsen, S. *Energy and Buildings*, 2013, 64, 309–316.

This paper evaluates the daylighting performance of a prototype external dynamic shading and daylight-redirecting system, and the main focus is on the performance simulation. The demonstration project was carried out on a building with an open-plan office. Part of the original façade was replaced with the prototype façade. This layout allowed the use of the same orientation and surroundings for both façades. The working plane illuminance was measured over several months and the measurements were accompanied with annual daylight simulations. The prototype system improved the daylighting conditions compared to the original system. The visual comfort was evaluated by glare analysis and the redirected daylight did not cause an additional discomfort glare. The higher utilization of daylight can save 20% of the lighting energy. The thermal insulation of the fenestration was maintained, with slightly increased solar gains, but without producing an excessive overheating.

14/02136 Preparation and evaluation of thermal enhanced silica fume by incorporating organic PCM, for application to concrete

Jeong, S.-G. *et al. Energy and Buildings*, 2013, 62, 190–195.

Silica fume has been used as a replacement for cement, due to its high early compressive strength, high tensile and flexural strength, high bond strength, and enhanced durability of concrete. This study examined enhanced thermal performances of silica fume by incorporating organic phase change material (PCMs), for applying to concrete. Three kinds of organic PCMs were incorporated into the silica fume. The silica fume/PCM composites were prepared by the vacuum impregnation method. Because silica fume has a high porous structure compared to cement, it is useful to incorporate the PCM, to enhance its thermal storage performance. The characteristics of the composites were determined by using various analytical techniques. Scanning electron microscope morphology showed the micro-structure of silica fume/PCM. Also, thermal properties were examined by differential scanning calorimetry and thermogravimetric analyses; and the chemical bonding of the composite was determined by Fourier-transform infrared spectroscopy analysis.

14/02137 Studies on the operation of trap filters and oscillators systems based on ceramic resonators at the cryogenic temperatures

El-Ghanam, S. M. *et al. Cryogenics*, 2013, 57, 88–94.

This study investigated the temperature dependence of the applications of piezo PZT ceramic resonators down to 93 K in oscillators and filters circuits inside a frequency range of 400 kHz–4.0 MHz. For both systems, their waveforms were plotted at different temperature values ranging from room level (293 K) down to (93 K). From which, it is clearly shown that, cryogenic temperature effect on the operation of the trap filter system was shown to increase the voltage value at stop-band from 1.40 V, measured at 293 K, up to 4.40 V. The rise and fall times of the square wave oscillator were shown to increase slightly with temperature decreasing. Initial values of 92.3 ns, and 85.8 ns, measured at 293 K, were observed to increase up to 106 and 107 ns, measured at 93 K, respectively, while the signal output was kept constant. But for the sine-wave oscillator, its frequency, and output voltage were shown decrease as the temperature decreases.

14/02138 The effect of 24c-site (A) cation substitution on the tetragonal–cubic phase transition in $Li_{7-x}La_{3-x}A_xZr_2O_{12}$ garnet-based ceramic electrolyte

Rangasamy, E. *et al. Journal of Power Sources*, 2013, 230, 261–266.

The garnet-type ceramic electrolyte of nominal composition $Li_7La_3Zr_2O_{12}$ can exist in the tetragonal and cubic form. This paper investigates the tetragonal to cubic phase transition based on supervalent cation substitution on the 24c site typically occupied by La (3+) in the garnet structure. Ce (4+) was selected as the super-valent cation represented as x in $Li_{7-x}La_{3-x}Ce_xZr_2O_{12}$. The doping study showed that cubic LLZO was stabilized for $Ce \geq 0.2$. These data agree with most literature reports suggesting that the creation of Li vacancies, while maintaining oxygen stoichiometry, is necessary to stabilize cubic

LLZO. Moreover, this work suggests a critical Li vacancy concentration (0.12–0.4 mol per mole of $Li_7La_3Zr_2O_{12}$) is necessary to stabilize cubic LLZO. While the addition of Ce stabilized cubic LLZO, the total ionic conductivity (0.014 mS cm^{-1}) was considerably lower compared to Al and Ta doped LLZO (0.4–0.9 mS cm^{-1}, respectively). The lower conductivity is likely due to CeO_2 precipitation at grain boundaries.

14/02139 Towards biofuel combustion with an easily extruded clay as a natural catalyst
Tian, Z.-Y. *et al. Applied Energy*, 2013, 107, 149–156.
The present work aims to investigate an innovative application of natural clay as a catalyst for biofuel combustion. The mineralogical, chemical, thermal and textural characterizations of the natural clay suggest an intrinsic catalytic potential without any prior treatment. The catalytic performance was studied with respect to the combustion of *n*-butanol as a representative biofuel using different forms of the natural clay: fine powder, pressed pellets and extruded honeycomb monoliths. No major difference was found among these forms regarding texture, morphology and stability. In terms of performance, this clay proved competitive relative to cobalt oxide spinel, which is one of the most reactive non-noble transition metal oxides. The significant amount of naturally occurring transition metals such as iron and some elements considered as promoters in the clay were proposed to account for the catalytic properties. A systematic investigation of the catalytic performance of the clay as a function of the equivalence ratio and of the total flow rate was performed using gas-phase Fourier transform infrared spectroscopy. Increase of the equivalence ratio at a fixed flow rate yielded a lower catalytic performance toward *n*-butanol combustion producing a consequent fraction of carbon monoxide and ethylene. At a constant equivalence ratio of 0.6, the performance of the clay was not affected by increasing the total inlet flow rate up to 30 sccm. These findings may initiate the development of a new catalyst for biofuel combustion based on relatively low-cost and abundantly available raw materials such as the natural clay investigated here.

14/02140 Use of Coandă nozzles for double glazed façades forced ventilation
Valentín, D. *et al. Energy and Buildings*, 2013, 62, 605–614.
Fans are the most widespread system used to implement forced convection ventilation for double-glazed façades (DGF). However, the implementation of fans in a façade require an electrical supply for the motors, solid supports for the fans, and the installation has to meet fire safety regulations required by local laws. These facts, added to the need of a regular maintenance programme for the fans and the possibility of noise and vibration generated by the moving parts of these equipment, might increase the final cost of the façade and reduce the comfort inside the building. In this paper the feasibility of using nozzles for DGF ventilation is evaluated. The nozzles selected for this study are based on the Coandă effect. For this investigation, a computational fluid dynamics model was used to simulate a Coandă nozzle. The modelled nozzle was simulated for different flow rate conditions and velocity and pressure fields obtained in the nozzle outlet were imposed as an inlet boundary condition in an upper crossed lateral ventilation model for a DGF. Results obtained for heat flux, and reductions in solar gain loads for different operating conditions were obtained and compared against previous results for vertical and horizontal DGF ventilation in a similar geometry.

14/02141 Waste lubricating oil treatment by extraction and adsorption
Mohammed, R. R. *et al. Chemical Engineering Journal*, 2013, 220, 343–351.
In this work, the recovery of base oils from waste lubricants was investigated using a novel combination of solvent extraction and adsorption on solids. The performance of six extracting solvents (*n*-hexane, 1-butanol, petroleum ether, 1-hexanol, carbon tetrachloride and acetone) was evaluated experimentally. Solvent to oil ratios from 1 : 1 to 4 : 1 were also examined. This research has studied the effect of the use of KOH to enhance flocculation. The results show that 1-butanol achieved the best performance with the maximum percentage sludge removal, followed by n-hexane, petroleum ether, 1-hexanol, carbon tetrachloride and acetone. The percentage of oil sludge was found to increase with the increase of solvent-to-oil ratio until it reached the maximum at the ratio of 3 : 1. The application of an adsorption process using different adsorbent materials was investigated. Adsorbent materials such as almond shell, walnut shell, eggshell and acid-activated clay which were prepared locally were used. It was found that the acid activated clay was able to give the best conditions for treating the waste oil followed by the almond shell powder. The results from the test showed that, viscosity increased from 38.3 cst for used lube oil to 85 cst for acid/clay treatment and the flash point increase from 178 to 238 °C, while the density decreased from 912 to 896 kg/m^3, the pour point from −6 to −13.2 °C and colour from 0.53 to 0.12. Other results from the different tests showed varying degrees of improvement with the best results obtained using the acid/clay treatment.

13 ALTERNATIVE ENERGY SUPPLIES

Biofuels and bioconversion energy

14/02142 A GIS based assessment of bioenergy potential in England within existing energy systems
Thomas, A. *et al. Biomass and Bioenergy*, 2013, 55, 107–121.
This paper presents an analysis of the spatial supply and demand relationships for biomass energy potential for England, using geographical information system (GIS) mapping techniques. Due to energy use and cost of biomass feedstock transportation, the spatial relationship between potential supply and demand is crucial to efficient usage of this distributed feedstock. Previous studies have identified potential for biomass generation at individual sites, according to local factors dictating viable transport distances and costs. The research presented here necessarily takes a more generalized approach, to allow national scale assessment of capability to meet fixed location demands, and quantify theoretical potential generation under relevant scenarios. The approach is illustrated for England, although techniques are applicable elsewhere when suitable data are available. Mapping for England indicates that of the 2,521,996 ha viable for cultivation of *Miscanthus*, 1,998,435 ha are within 25 km of the identified potential end uses of feedstock, and 2,409,541 ha are within 40 km. Potential generation exceeds the 2020 UK biomass generation target of 259 PJ, whichever radius is applied. However, predictions assume *Miscanthus* cultivation at all appropriate sites, and no policy interventions to limit transport distance. Results from national scale analysis may be useful in informing government decisions, for example to identify impacts on total generation potential of incentives affecting decisions on allocation of overlap feedstock. Variation in greenhouse gas balance and environmental impacts between cultivation sites creates spatial variation in benefits of bioenergy, which should be taken into account in addition to the spatial relationship between supply and demand.

14/02143 Biodiesel from waste cooking oils via direct sonication
Gude, V. G. and Grant, G. E. *Applied Energy*, 2013, 109, 135–144.
This study investigates the effect of direct sonication in conversion of waste cooking oil into biodiesel. Waste cooking oils may cause environmental hazards if not disposed properly. However, waste cooking oils can serve as low-cost feedstock for biodiesel production. Ultrasonics, a non-conventional process technique, was applied to directly convert waste cooking oil into biodiesel in a single step. Ultrasonics transesterify waste cooking oils very efficiently due to increased mass/heat transfer phenomena and specific thermal/athermal effects at molecular levels. Thus, energy and chemical consumption in the overall process is greatly reduced compared to conventional biodiesel processes. Specific to this research, thermal effects of ultrasonics in transesterification reaction without external conventional heating along with effects of different ultrasonic, energy intensities and energy density are reported. Optimization of process parameters such as methanol to oil ratio, catalyst concentration and reaction time are also presented. It was observed that small reactor design such as plug-flow or contact-type reactor design may improve overall ultrasonic utilization in the transesterification reaction due to increased energy density and ultrasonic intensity.

14/02144 Biomass production from the U.S. forest and agriculture sectors in support of a renewable electricity standard
White, E. M. *et al. Energy Policy*, 2013, 58, 64–74.
Production of renewable energy from biomass has been promoted as means to improve greenhouse gas balance in energy production, improve energy security, and provide jobs and income. However, uncertainties remain as to how the agriculture and forest sectors might jointly respond to increased demand for bioelectricity feedstocks and the potential environmental consequences of increased biomass production. This study uses an economic model to examine how the agriculture and forest sectors might combine to respond to increased demands for bioelectricity under simulated future national-level renewable electricity standards. Both sectors are projected to contrib-

ute biomass, although energy crops, like switchgrass, produced on agriculture land are projected to be the primary feedstocks. At the highest targets for bioelectricity production, increased conversion of forest to agriculture land in support of agriculture biomass production is projected. Although land conversion takes place in response to renewable electricity mandates, only minor increases in forest and agriculture emissions are projected. Similarly, crop prices were projected to generally be stable in the face of increased bioelectricity demand and displacement of traditional agriculture crops.

14/02145 Biorefineries for the production of first and second generation ethanol and electricity from sugarcane

Dias, M. O. S. *et al. Applied Energy*, 2013, 109, 72–78.

Sugarcane trash and bagasse, lignocellulosic materials obtained during sugarcane harvesting and processing, may be used as fuels for electricity production and/or as feedstock for second generation ethanol. If electricity prices are favourable, more lignocellulosic material may be diverted for production of steam and electricity, and vice versa when ethanol prices are more attractive. Therefore, some flexibility to divert bagasse and trash for either second-generation ethanol or electricity production might help to maximize revenues. An analysis of the integrated first and second- generation ethanol production process from sugarcane is presented, evaluating its flexibility. A flexible biorefinery may offer economic and environmental advantages over the conventional biorefineries with fixed production capacity.

14/02146 Comparison of biogas upgrading performances of different mixed matrix membranes

Ozturk, B. and Demirciyeva, F. *Chemical Engineering Journal*, 2013, 222, 209–217.

In this study composite membranes were manufactured by introducing zeolite 3A, 4A and 5A within polyimide (PI) and polyetherimide (PEI) in order to increase their separation performances for the gaseous mixture of CO_2 and CH_4 which are main components of the biogas. The effects of annealing temperatures, zeolite loadings, feed pressures and mixed gas and biogas feedings on the separation of CO_2–CH_4 by membranes were investigated. It has also investigated that whether there is a relation between gas sorption capacity and separation performances of membranes manufactured. Membranes were characterized by differential scanning calorimetry, thermogravimetic analysis and scanning electron microscopy analysis. The pure gas permeation and the mixed gas or biogas separation experiments indicated that the mixed matrix membranes (MMMs) prepared by introducing zeolite 4A into PI is a suitable candidate for CO_2/CH_4 separation and/or methane enrichment from biogas. Zeolite loading into PEI increased the CO_2 and CH_4 permeabilities more than PI/zeolite-MMMs showed. But, the higher the zeolite loadings caused the lower the ideal CO_2/CH_4 selectivities for PEI/zeolite-MMMs at all the feed pressures applied. The results also showed that there is a partial relation between gas permeability and sorption capacity of membranes used. The results of biogas separation experiments showed that the CO_2 content in the permeated gas increased as much as 95% at 3 bar feed pressure. The highest CO_2 content in the permeated gas was obtained when PI/4A-MMM was used, and followed by PI/3A, pure PI, PI/5A, pure PEI, PEI/5A, PEI/4A and PEI/3A.

14/02147 Design methodology for bio-based processing: biodiesel and fatty alcohol production

Simasatitkul, L. *et al. Computers & Chemical Engineering*, 2013, 57, 48–62.

A systematic design methodology is developed for producing multiple main products plus side products starting with one or more bio-based renewable source. A superstructure that includes all possible reaction and separation operations is generated through thermodynamic insights and available data. The number of alternative processes is systematically reduced through a screening procedure until only feasible alternatives are obtained. As part of the methodology, process intensification involving reaction–separation tasks is also considered to improve the design by shifting the equilibrium reactions. Economic analysis and net present value are determined to find the best economically and operationally feasible process. The application of the methodology is presented through a case study involving biodiesel and fatty alcohol productions.

14/02148 Development of an effective acidogenically digested swine manure-based algal system for improved wastewater treatment and biofuel and feed production

Hu, B. *et al. Applied Energy*, 2013, 107, 255–263.

An effective semi-continuous process was developed to grow a locally isolated green microalga *Chlorella* sp. on acidogenically digested swine wastewater in bench scale for improved algal biomass production and waste nutrient removal using central composite design (CCD). The influences of two key parameters, namely wastewater dilution rate (DR) and hydraulic retention time (HRT), on algal biomass productivity and nutrient removal rates were investigated. The optimal parameters estimated from the significant second-order quadratic models ($p < 0.05$) were right-fold DR and 2.26-d HRT. The cultivating experiment in a bench-scale multi-layer photobioreactor with the optimized conditions achieved stable algal productivity and nutrient removal rates, which fitted the predictive models well. Moreover, relatively high and stable protein and lipid contents (58.78% and 26.09% of the dry weight, respectively) were observed for the collected algae sample, indicating the suitability of the algal biomass as ideal feedstock for both biofuel and feed production.

14/02149 Energetic and environmental performance of three biomass upgrading processes integrated with a CHP plant

Kohl, T. *et al. Applied Energy*, 2013, 107, 124–134.

In order to react to future expected increased competition on restricted biomass resources, communal combined heat and power (CHP) plants can be integrated with biomass upgrading processes that add valuable products to the portfolio. In this paper, outgoing from a base case, the retrofit integration of production of wood pellets (WPs), torrefied wood pellets (TWPs) and wood fast pyrolysis slurry (PS) with an existing wood-fired CHP plant was simulated. Within the integration concept, free boiler capacity during times of low district heat demands is used to provide energy for the upgrading processes. By detailed part-load modelling, critical process parameters are discussed. With help of a multiperiod model of the heat duration curve, the work further shows the influence of the integration on plant operating hours, electricity production and biomass throughput. Environmental and energetic performance is assessed according to European standard EN 15603 and compared to the base case as well as to stand-alone production in two separate units. The work shows that all three integration options are well possible within the operational limits of the CHP plant. In summary, this work shows that integration of WP, TWP and PS production from biomass with a CHP plant by increasing the yearly boiler workload leads to improved primary energy efficiency, reduced CO_2 emissions, and, when compared to stand-alone production, also to substantial fuel savings.

14/02150 Global assessment of research and development for algae biofuel production and its potential role for sustainable development in developing countries

Adenle, A. A. *et al. Energy Policy*, 2013, 61, 182–195.

The possibility of economically deriving fuel from cultivating algae biomass is an attractive addition to the range of measures to relieve the current reliance on fossil fuels. Algae biofuels avoid some of the previous drawbacks associated with crop-based biofuels as the algae do not compete with food crops. The favourable growing conditions found in many developing countries has led to a great deal of speculation about their potentials for reducing oil imports, stimulating rural economies, and even tackling hunger and poverty. By reviewing the status of this technology, the authors suggest that the large uncertainties make it currently unsuitable as a priority for many developing countries. Using bibliometric and patent data analysis, it was found that many developing countries may lack the human capital to develop their own algae industry or adequately prepare policies to support imported technology. Also, the authors discuss the potential of modern biotechnology, especially genetic modification (GM) to produce new algal strains that are easier to harvest and yield more oil. Controversy surrounding the use of GM and weak biosafety regulatory system represents a significant challenge to adoption of GM technology in developing countries. A range of policy measures are also suggested to ensure that future progress in algae biofuels can contribute to sustainable development.

14/02151 Harvesting of marine microalgae by electroflocculation: the energetics, plant design, and economics

Lee, A. K. *et al. Applied Energy*, 2013, 108, 45–53.

Microalgae have the potential to be the feedstock for biofuels and laboratory scale electroflocculation was studied as a harvesting technique for marine microalgae. The effects of the electrode separation and mechanical mixing on the energy consumption were also assessed. Results were used to design a commercial scale electroflocculation plant for the estimation of the harvesting cost. By combining electroflocculation with mixing and settling, an overall energy consumption of $0.33\,MJ\,m^{-3}$ has been achieved. On a large scale, the mixing can be made energy efficient by the use of a baffled hydraulic mixer. The total cost for the harvesting, including electrical energy, electrode metal dissolution and capital depreciation, is estimated to be $\$0.19\,kg^{-1}$ of the ash free dry mass. Hence, electroflocculation has the potential to be more economical than other harvesting techniques for marine microalgae.

14/02152 Hemp: a more sustainable annual energy crop for climate and energy policy

Finnan, J. and Styles, D. *Energy Policy*, 2013, 58, 152–162.

The objective of this study was to compare the fuel-chain greenhouse gas balance and farm economics of hemp grown for bioenergy with two perennial bioenergy crops, *Miscanthus* and willow, and two more traditional annual bioenergy crops, sugar beet and oil seed rape (OSR). The greenhouse gas (GHG) burden of hemp cultivation is intermediate between perennial and traditional annual energy crops, but net fuel chain GHG abatement potential of 11 t/CO_2 eq./ha/year in the mid-yield estimate is comparable to perennial crops, and 140% and 540% greater than for OSR and sugar beet fuel chains, respectively. Gross margins from hemp were considerably lower than for OSR and sugar beet, but exceeded those from *Miscanthus* when organic fertilizers were used and in the absence of establishment grants for the latter crop. Extrapolated up to the European Union scale, replacing 25% of OSR and sugar beet production with hemp production could increase net GHG abatement by up to 21 Mt CO_2eq./year. Hemp is a considerably more efficient bioenergy feedstock than the dominant annual energy crops. Integrated into food crop rotations, hemp need not compete with food supplies, and could provide an appealing option to develop more sustainable non-transport bioenergy supply chains.

14/02153 Multi-scale models for the optimization of batch bioreactors

Liew, E. W.-T. *et al. Chemical Engineering Science*, 2013, 95, 257–266.

Process models play an important role in the bioreactor design, optimization and control. In previous work, the bioreactor models have mainly been developed by considering the microbial kinetics and the reactor environmental conditions with the assumption that the ideal mixing occurs inside the reactor. This assumption is relatively difficult to meet in the practical applications. This study proposes a new approach to the bioreactor modelling by expanding the so-called Herbert's microbial kinetics (HMK) model so that the developed models are able to incorporate the mixing effects via the inclusion of the aeration rate and stirrer speed into the microbial kinetics. The expanded models of Herbert's microbial kinetics allow us to optimize the bioreactor's performances with respects to the aeration rate and stirrer speed as the decision variables, where this optimization is not possible using the original HMK model of microbial kinetics. Simulation and experimental studies on a batch ethanolic fermentation demonstrates the use of the expanded HMK models for the optimization of bioreactor's performances. It is shown that the integration of the expanded HMK model with the computational fluid dynamics model of mixing, as a kinetics multi-scale model, is able to predict the experimental values of yield and productivity of the batch fermentation process accurately (with less than 5% errors).

14/02154 Optimal processing pathway for the production of biodiesel from microalgal biomass: a superstructure based approach

Rizwan, M. *et al. Computers & Chemical Engineering*, 2013, 58, 305–314.

This study proposes a mixed integer non-linear programming (MINLP) model for superstructure-based optimization of biodiesel production from microalgal biomass. The proposed superstructure includes a number of major processing steps for the production of biodiesel from microalgal biomass, such as the harvesting of microalgal biomass, pretreatments including drying and cell disruption of harvested biomass, lipid extraction, transesterification, and post-transesterfication purification. The proposed model is used to find the optimal processing pathway among the large number of potential pathways that exist for the production of biodiesel from microalgae. The proposed methodology is tested by implementing on a specific case with different choices of objective functions. The MINLP model is implemented and solved in GAMS using a database built in Microsoft Excel. The results showed that, depending on the objective functions that have been chosen, different optimal processing pathways were found. The proposed optimization model enables alternative processing pathways to be considered under different potential objectives. This method is a systematic way for determining an optimal processing pathway and has the capacity to screen through all potential processing alternatives to locate the promising ones under various possible objectives. Based on the obtained information, a detailed process flowsheet can be synthesized for a more detailed economic evaluation.

14/02155 Options analysis for long-term capacity design and operation of a lignocellulosic biomass refinery

Sharma, P. *et al. Computers & Chemical Engineering*, 2013, 58, 178–202.

The growth of the lignocellulosic fuels has been hindered by technological and market uncertainty. This paper optimizes strategic investment decisions by prospective biobased fuel and chemical enterprises. A real options-based stochastic integer programming model is developed in this paper. The authors model a hypothetical, vertically integrated lignocellulosic enterprise that produces cellulosic ethanol and biosuccinic acid. Uncertainty is represented in bioproduct demands and prices. Strategic options including investment in research and development, investments in a flexible production platform and deferral of project investment are modelled. A hypothetical market model is also developed to correlate crude oil prices with the evolution of bioproduct markets. The discounted value of equity-free cash flows is optimized. The optimal results include multiple capacity design plans based on the long-term evolution of bioproduct markets. Monte Carlo simulations are also conducted to quantify the risk adjusted net present values and returns on investment for the optimal capacity design trajectories.

14/02156 Potentialities of energy generation from waste and feedstock produced by the agricultural sector in Brazil: the case of the state of Paraná

de Fátima dos Santos Ribeiro, M. and Raiher, A. P. *Energy Policy*, 2013, 60, 208–216.

The state of Paraná contributes significantly to the Brazilian production of sugar cane, ethanol, soybeans and pigs. In addition to the current production of ethanol, the state has a huge potential for electricity, biodiesel and biogas production. This paper presents an overview of the current situation regarding energy generation from the agricultural sector in the state, an assessment of the potentialities of energy generation from sugar cane residues and pig agricultural chains, as well as an analysis of the socioeconomic factors underlying the availability of feedstock for biodiesel production. This study has shown that it is possible to expand the energy supply in the state using residual biomass from the sugar cane and pig production. On the other side, the biodiesel production increase in the state will depend on the expansion in the consumption of products that use the cake as raw material; the increase in the feedstock availability other than canola, castor beans and sunflower; the increase of the number of family farmers as feedstock providers, so as to ensure access for biodiesel producers to the social fuel stamp.

14/02157 Scenarios for biofuel demands, biomass production and land use – the case of Denmark

Larsen, L. E. *et al. Biomass and Bioenergy*, 2013, 55, 27–40.

The land potential for producing biomass for bioenergy purposes has been highly debated in recent years. This paper analyses the possibilities and consequences for land use and agricultural production of biofuel production in Denmark based on domestic wheat and rape under specific scenario conditions for the period 2010–2030. The potential is assessed for a situation where policy targets for renewable energy carriers in the transport sector is reached using biofuels, and where second-generation ethanol increasingly substitutes first-generation ethanol. Three scenarios are developed and evaluated: a baseline, an alternative scenario allowing continuous growth in the now dominant livestock branch and a biofuel scenario assuming that efforts to achieve self-sufficiency in biofuel displaces part of the domestic production of fodder. Results show that the biofuel demand could be met in 2020; but only if current rape oil production is used to satisfy local bio-diesel demand. It would also imply that the Danish bio-diesel export currently supplying a minor part of the German fuel market would seize. In 2030, however, only about 60% of the biofuel demand would be covered by self-sufficiency. If biofuels were to displace animal production to make up for this, a reduction of the pig production between 10% and 20% would result. Efficiency increases across production branches would allow the animal production to continue unaffected if about half of the rape oil produced for other purposes is utilized.

14/02158 Short rotation forestry feedstock: influence of particle size segregation on biomass properties

Jacob, S. *et al. Fuel*, 2013, 111, 820–828.

Short rotation forestry (SRF) is a promising feedstock for production of biofuels via the thermochemical route. Five poplar biomasses (SRF of different clones and ages, and debarked wood) were ground and separated into three particle size fractions: <0.2, 0.2–0.4 and >0.4 mm. The characterization of these samples was performed to evaluate the quality and homogeneity of SRF feedstocks. Some major properties related to thermochemical processes were measured: chemical composition, organic and inorganic elemental compositions. The heterogeneity in SRF feedstock properties, resulting from high bark content, appeared to be transferred to particle size fractions. The results obtained highlighted that fine particles <0.2 mm had very specific properties, close to those of bark. The removal of this fraction would result in a more homogeneous feedstock, avoiding the issue caused by segregation risk for process stability. Such removal of small particles would also modify the biomass properties by reducing bark amount, improving the suitability of SRF feedstock for thermochemical conversion.

14/02159 Straw use and availability for second generation biofuels in England

Glithero, N. J. *et al. Biomass and Bioenergy*, 2013, 55, 311–321.

Meeting European Union targets for renewable transport fuels by 2020 will necessitate a large increase in bioenergy feedstocks. Although deployment of first-generation biofuels has been the major response to meeting these targets they are subject to wide debate on their sustainability leading to the development of second-generation technologies which use lignocellulosic feedstocks. Second-generation biofuel can be subdivided into those from dedicated bioenergy crops (DESGB), e.g. *Miscanthus*, or those from co-products (CPSGB) such as cereal straw. Potential supply of cereal straw as a feedstock for CPSGB's is uncertain in England due to the difficulty in obtaining data and the uncertainty in current estimates. An on-farm survey of 249 farms (cereal, general cropping and mixed) in England was performed and linked with farm business survey data to estimate current straw use and potential straw availability. No significant correlations between harvested grain and straw yields were found for wheat and oilseed rape and only a weak correlation was observed for barley. In England there is a potential cereal straw supply of 5.27 Mt from arable farm types; 3.82 Mt are currently used and 1.45 Mt currently chopped and incorporated. If currently chopped and incorporated cereal straw from arable farm types was converted into bioethanol, this could represent 1.5% of the UK petrol consumption by energy equivalence. The variations in regional straw yields ($t\,ha^{-1}$) have a great effect on the England supply of straw and the potential amount of bioethanol that can be produced.

14/02160 The economics of oil, biofuel and food commodities

Bahel, E. *et al. Resource and Energy Economics*, 2013, 35, (4), 599–617.

This study considers the effects on the food price of introducing biofuels as a substitute for fossil fuel in the energy market. Energy is supplied by a price-leading oil cartel and a competitive fringe of farmers producing biofuel. Biofuel production shares a finite land resource with food production. A positive relationship results between energy and food prices. The authors establish that the equilibrium price of food will be growing as long as the oil stock is being depleted, and beyond if demand is growing. An analysis of the effects of the productivity of land use in either the food or the biofuel sectors is carried out. It is shown that, with a highly inelastic demand for food, an increase in the productivity of land in agriculture will decrease the price of food in the short-run, only to increase it in the long-run as the stock of fossil fuel is depleted.

14/02161 Thermo-economic evaluation and optimization of the thermo-chemical conversion of biomass into methanol

Peduzzi, E. *et al. Energy*, 2013, 58, 9–16.

In a carbon- and resource-constrained world, the thermo-chemical conversion of lignocellulosic biomass into fuels and chemicals is regarded as a promising alternative to fossil resource-derived products. Methanol is one potential product that can be used for the synthesis of various chemicals or as a fuel in fuel cells and internal combustion engines. This study focuses on the evaluation and optimization of the thermodynamic and economic performance of methanol production from biomass by applying process integration and optimization techniques. The results reveal the importance of the energy integration and in particular of the cogeneration of electricity for the efficient use of biomass.

14/02162 Threshold herd size for commercial viability of biomass waste to energy conversion systems on rural farms

Namuli, R. *et al. Applied Energy*, 2013, 108, 308–322.

The main contribution from the research undertaken is the specification of the threshold herd size at which biomass waste-to-energy conversion systems become commercially viable. The threshold herd sizes at which these systems become commercially viable have been determined, as 80 dairy cows and 1200 pigs. This was done by calculation of the net present values of these systems for different herd sizes. Optimization of the biomass waste to energy conversion system was carried out prior to calculation of its net present value. The scientific significance of the research is the determination of the commercial viability of a complex biomass waste to energy conversion system by solving a non-linear, complex optimization problem, with non-convex constraints, using the Tabu search technique. A sample farm in Quebec province with a herd size of 240 cows was analysed to validate the findings. The results of the optimization for the sample farm showed that the farm could obtain a revenue of $26,525 annually, from the sale of electricity to the utility company throughout the year. It is recommended that a net metering contract that allows the sale of electricity in excess of the net energy demand over a 24-month period be considered by the utility company. It is also recommended that the net metering contract should apply to renewable energy generators who generate electricity in excess of their demand or in excess of 50 kW. Further work in this area can be done on determination of commercial viability of biomass waste-to-energy conversion systems in other regions of Canada, and for other conditions, for example, the use of subsidies in Quebec.

Geothermal energy

14/02163 A new computational modeling to predict the behavior of earth-air heat exchangers

da Silva Brum, R. *et al. Energy and Buildings*, 2013, 64, 395–402.

The use of renewable energy sources to improve the thermal conditions of built environments and hence decreasing the consumption of conventional energy is an important aspect to design a sustainable building. Within this context, it is possible to harness the solar energy that reaches the Earth's surface and is stored by the soil as thermal energy. To do so, the earth–air heat exchanger (EAHE) device can be employed, consisting of a buried duct through which the external ambient air is insufflated. The flowing air exchanges heat with surround soil, and leaves the device with a milder temperature compared to its input temperature. The main goal of this work was to present a new computational modelling to predict the thermal behaviour of EAHE. This new numerical model has the advantage of needing a lower computational effort, allowing the study about the influence of operational and constructive parameters, as well as, the application of geometric optimization methods in EAHE. A case study was developed where influence of the installation depth in the thermal potential of an EAHE was investigated. The results are in agreement with those found in literature; however they were obtained with a reduction in processing time of almost 45%.

14/02164 Development of a geothermal based integrated system for building multigenerational needs

Ratlamwala, T. A. H. and Dincer, I. *Energy and Buildings*, 2013, 62, 496–506.

The present study develops a new integrated geothermal-based system, comprising of quadruple flash power plant (QFPP), quadruple effect absorption cooling system (QEACS), electrolyser and air-conditioning process (cooling with dehumidification) for building applications. The system is designed to generate six outputs namely, power, hot water, heating, cooling, hydrogen and dry air to meet the building needs. The system analysis is carried out through energy and exergy, and parametric studies are carried out to see the effect of variation in geothermal pressure at state f2, geothermal liquid temperature, relative humidity and evaporator load on performance of the integrated system. Illustrations are also provided to display the effect of variation in geothermal liquid pressure at state f2 and geothermal liquid temperature on the exergy efficiencies as the number of output increases. The results show that the exergy efficiency increases from 0.20 to 0.28 with increase in geothermal liquid temperature from 450 to 500 K and number of generations from single to hextuple generation. An optimization study is also carried out to find the highest possible exergy efficiency and the lowest possible exergy destruction of the hextuple generation system.

14/02165 Distributed thermal response tests on pipe-in-pipe borehole heat exchangers

Acuña, J. and Palm, B. *Applied Energy*, 2013, 109, 312–320.

Borehole thermal energy storage systems typically use U-pipe borehole heat exchangers (BHE) having borehole thermal resistances of at least 0.06 K m/W. Obviously, there is room for improvement in the U-pipe design to decrease these values. Additionally, there is a need for methods of getting more detailed knowledge about the performance of BHEs. Performing distributed thermal response tests (DTRT) on new proposed designs helps to fill this gap, as the ground thermal conductivity and thermal resistances in a BHE can be determined at many instances in the borehole thanks to distributed temperature measurements along the depth. In this paper, results from three heat injection DTRTs carried out on two coaxial pipe-in-pipe BHEs at different flow rates are presented for the first time. The tested pipe-in-pipe geometry consists of a central tube inserted into a larger external flexible pipe, forming an annular space between them. The external pipe is pressed to the borehole wall by applying a slight overpressure at the inside, resulting in good thermal contact and at the same time opening up for a novel method for measuring the borehole wall temperature *in situ*, by squeezing a fibre optic cable between the external pipe and the borehole wall. A reflection about how to calculate borehole thermal resistance in pipe-in-pipe BHEs is presented. Detailed fluid and borehole wall temperatures along the depth during the whole duration of the DTRTs allowed to calculate local and effective borehole thermal resistances and ground thermal conductivities. Local thermal resistances were found to be almost

negligible as compared to U-pipe BHEs, and the effective borehole resistance equal to about 0.03 K m/W. The injected power was found to be almost evenly distributed along the depth.

14/02166 Experimental and modeling analysis of a ground source heat pump system

Montagud, C. *et al. Applied Energy*, 2013, 109, 328–336.

This paper presents the evaluation of the performance of a ground source heat pump system monitored plant providing heating/cooling to an office building located in the Universitat Politècnica de València in Spain. The system was designed using GLHEPRO software and it has been monitored since 2005. Once a ground source heat pump has been designed, it is important to analyse its performance along the years after its construction and check whether the design was appropriate and the simulation predictions were consistent with real experimental measurements. This paper first presents the impact of the GSHP system in the ground thermal response. The simulations obtained in GLHEPRO software will be analysed and compared to experimental measurements. The second purpose of this work is to compare the performance simulation results of a complete ground source heat pump system model built in TRNSYS, with the experimental measurements which have been registered and collected for one cooling day. Numerical predictions and experimental results are compared and discussed.

14/02167 Exploration of geothermal systems using hyperspectral thermal infrared remote sensing

Reath, K. A. and Ramsey, M. S. *Journal of Volcanology and Geothermal Research*, 2013, 265, 27–38.

Visible near infrared (VNIR), short-wave infrared (SWIR) and thermal infrared (TIR) remote sensing has long been used for geothermal exploration. Specific focus on the TIR region (8–12 μm) has resulted in major-rock-forming mineral classes being identified and their areal percentages to be more easily mapped due in part to the linear mixing behaviour of TIR emission. To understand the mineral compositional and thermal distribution of active geothermal surfaces systems, hyperspectral TIR data from the spatially enhanced broadband array spectrograph system (SEBASS) airborne sensor were acquired over the Salton Sea, CA geothermal fields by the Aerospace Corporation on 26 March 2009 and 6 April 2010. SEBASS collects 128 wavelength channels at ~1 m spatial resolution. Such high-resolution data are rarely available for this type of scientific analysis and enabled the identification of rare mineral assemblages associated with the geothermally active areas. One surface unit with a unique spectrum, believed to be a magnesium sulfate of unknown hydration state, was identified for the first time in the SEBASS data. The abundance and distribution of this mineral varied between 2009 and 2010 likely due to the precipitation conditions. Data obtained by the SEBASS sensor were also regressed to the 32-channel spectral resolution of the mineral and gas identifier (MAGI) airborne sensor in order to test sensitivity limits. At this lower spectral resolution, all surface minerals were still effectively identified and therefore validated data at MAGI resolution are still very effective for accurate surface compositional mapping. A similar approach used at active geothermal areas in other semi-arid regions around the world has the potential to better characterize transient mineralogy, identify 'indicators minerals', understand the influence of surface and ground water, and ultimately to locate new geothermal targets for future exploration. Furthermore, new MAGI data serve as an excellent precursor for future space-borne TIR data such as the system proposed for the hyperspectral infrared imager instrument.

14/02168 First in situ operation performance test of ground source heat pump in Tunisia

Naili, N. *et al. Energy Conversion and Management*, 2013, 75, 292–301.

The main purpose of this paper is to study the energetic potential of the deployment in Tunisia of the ground source heat pump system for cooling mode application. Therefore, a pilot GSHP system using horizontal ground heat exchangers (GHE) was installed and experimented in the Research and Technology Center of Energy (CRTEn), Borj Cédria. The experiment is conducted in a test room with a floor area of about 12 m^2. In the floor of the tested room is integrated a polyethylene exchanger used as a radiant floor cooling system. The experimental setup mainly includes the ground temperature, the temperature and flow rate of water circulating in the heat pump and the GHE, as well as the power consumption of the heat pump and circulating pumps. These experimental data are essentially used to evaluate the coefficient of performance of the heat pump (COP_{hp}) and the overall system (COP_{sys}) for continuous operation mode. The COP_{hp} and the COP_{sys} were found to be 4.25 and 2.88, respectively. These results reveal that the use of the ground source heat pump is very appropriate for Tunisian building cooling.

14/02169 High temperature metamorphism in the conductive boundary layer adjacent to a rhyolite intrusion in the Krafla geothermal system, Iceland

Schiffman, P. *et al. Geothermics*, 2014, 49, 42–48.

A rhyolite magma body within the Krafla geothermal system that was encountered at a depth of 2.1 km during drilling of the IDDP-1 borehole is producing high temperature metamorphism within a conductive boundary layer (CBL) in adjacent host rocks. Cuttings recovered during drilling within a few metres of the intrusive contact in IDDP-1 are mainly comprised of granoblastic hornfelses, the rock type which confirms the presence of the CBL at the base of the IDDP-1 bore hole. The two pyroxenes in these hornfelses record temperatures that are in the range of 800–950 °C. The minimum heat flow across the CBL is 23 W m^{-2}. Country rocks at distances beyond 30 m of the intrusive contact are essentially unaltered, implying that they have been emplaced very recently and/or as yet unaffected by hydrothermal fluid flow.

14/02170 Hydrogeochemical characterization and conceptual modeling of the Edremit geothermal field (NW Turkey)

Avşar, Ö. *et al. Journal of Volcanology and Geothermal Research*, 2013, 262, 68–79.

The Edremit geothermal field, with 42–62 °C discharge temperatures, is utilized for space heating. Alternation of permeable and impermeable units created two superimposed aquifers in the area: an upper unconfined and a lower confined. Water samples from 21 (hot–cold) wells were taken in this study. Eight of these wells penetrate the deeper confined aquifer, while 13 penetrate the shallower unconfined aquifer. Geochemical analyses revealed that $Na + K - SO_4$ (> 40 °C), $Ca - H\text{-}HCO_3$ (< 30 °C) and $Ca - SO_4$ (30–40 °C) waters occur. The $\delta^{18}O$-δD compositions point to a meteoric origin for all waters, while ^{14}C analyses suggest longer subsurface residence times for the hot waters, compared to the cold/warm waters. Chemical and isotopic compositions indicate that mixing and water–rock interaction are the possible subsurface processes. When silica and cation geothermometers are evaluated together with fluid-mineral equilibria calculations, a reservoir temperature range of 92–150 °C is evaluated. Saturation indices do not indicate a serious potential of scaling in the field. The hydrogeology of the study area is highly affected by faults. Infiltrated meteoric water percolates (down to 4.5 km depth) via deep seated step faults, becomes heated and ascends to the surface at the low lands, especially through intersection of buried, mid-graben faults. During its ascent, geothermal water invades the two superimposed aquifers where mixing between the hot and cold waters takes place.

14/02171 Modeling and assessment of the efficiency of horizontal and vertical ground heat exchangers

Florides, G. *et al. Energy*, 2013, 58, 655–663.

This paper describes the mathematical modelling of vertical and horizontal ground heat exchangers (GHEs) and compares their efficiency. The model used calculates the heat flow in the fluid, tubes, grout and ground. The vertical U-tube GHE is represented by two 100 m lines, embedded in four different types of ground with an additional bottom base. The horizontal GHE consists of four 50 m tube lines embedded in three ground layers. The initial ground temperature for all cases examined matches real data acquired in June at a location in Cyprus and the simulation results for the vertical GHE are validated using measured data showing very good agreement. Further simulations with the vertical GHE show that when the initial ground temperature rises, the mean temperature of the GHE fluid increases proportionally. Comparisons between horizontal and vertical GHEs reveal that under the same operating conditions and centre-to-centre distances of the tubes, the vertical GHE keeps a much lower mean temperature. Simulations for a horizontal GHE, for a 50-h of continuous operation period and 24 °C initial ground temperature, show that the mean fluid temperature can remain lower than that of the vertical GHE if the centre-to-centre distance of the tubes increases to 1 m.

14/02172 Reconstructing the geological and structural history of an active geothermal field: a case study from New Zealand

Milicich, S. D. *et al. Journal of Volcanology and Geothermal Research*, 2013, 262, 7–24.

The utilization of geothermal systems benefits from an understanding of the host-rock geology, locations and controls of permeability pathways, and the nature and timing of magmatic sources providing thermal energy. Kawerau geothermal field in the central Taupo volcanic zone (TVZ) of New Zealand is currently developed for electricity generation and direct uses of high-temperature steam to ~200 MW electrical output. The Kawerau geothermal system is hosted in a sequence of volcanic lithologies (tuffs, lavas and intrusive bodies) and sediments that overlie faulted Mesozoic metasedimentary (greywacke) basement. Identification of lithologies in the volcanic/sedimen-

tary sequence is challenging due to the levels of hydrothermal alteration and lithological similarities. A combination of detailed petrological investigations, consideration of the emplacement processes and greater certainty of crystallization or eruption ages through U–Pb age determinations on zircons is used to reconstruct the depositional and faulting evolution of the rocks hosting the currently active hydrothermal system. The oldest event inferred is faulting of the greywacke along north-west–south-east orientated, dominantly strike-slip structures to generate half-grabens that were filled with sediments, incorporating two dated ignimbrites (2.38 ± 0.05 and 2.17 ± 0.05 Ma). A 1.46 ± 0.01 Ma ignimbrite was deposited relatively evenly across the field, implying that any topographic relief was subdued at that time. Subsequent deposition of ignimbrites occurred in episodes around 1.0, 0.55–0.6 and 0.32 Ma, interspersed with thin sedimentary sequences that accumulated at average rates of $0.06\,mm\,yr^{-1}$. Andesite lavas from a buried composite cone occur as a conformable package between units dated at 1.0 and 0.6 Ma. Bodies of coherent rhyolite occur at multiple stratigraphic levels: two magma types with associated tuffs were emplaced as domes and sills at 0.36 ± 0.03 Ma, and a third type at 0.138 ± 0.007 Ma as dikes, and domes that are exposed at surface. The andesitic Putauaki composite cone south-west of the field first erupted around 8 ka, but earlier hydrothermal eruption breccias imply that magma was intruded to shallow depths as early as ~16 ka. Age data and associated correlations show that post-1.5 Ma normal faulting has accompanied episodic subsidence of the Kawerau area, with fault movement focused between north-east–south-west structures (associated with the geometry of the modern TVZ) and the reactivated north-west–south-east structures associated with most displacement in the area prior to 1.5 Ma. Contrasts between emplacement of coherent rhyolite as sills at 0.36 Ma and a dike at 0.138 Ma reflect a shift in orientation of the principal stress axes in response to initiation of the modern TVZ rifting regime. Most volcanic rocks at Kawerau are distally sourced from elsewhere in the TVZ but form local marker horizons that delineate topographic relief within the field, and additionally constrain past subsidence rates. Current rates of subsidence and thermal output at Kawerau are geologically recent features associated with latest Quaternary rifting processes (<50 ka) and emplacement of the magmatic system for Putauaki volcano (~16 ka) respectively.

14/02173 Spatial data analysis for exploration of regional scale geothermal resources

Moghaddam, M. K. *et al. Journal of Volcanology and Geothermal Research*, 2013, 266, 69–83.

Defining a comprehensive conceptual model of the resources sought is one of the most important steps in geothermal potential mapping. In this study, Fry analysis as a spatial distribution method and 5% well existence, distance distribution, weights of evidence (WofE), and evidential belief function methods as spatial association methods were applied comparatively to known geothermal occurrences, and to publicly-available regional-scale geoscience data in Akita and Iwate provinces within the Tohoku volcanic arc, in northern Japan. Fry analysis and rose diagrams revealed similar directional patterns of geothermal wells and volcanoes, NNW-, NNE-, NE-trending faults, hotsprings and fumaroles. Among the spatial association methods, WofE defined a conceptual model correspondent with the real world situations, approved with the aid of expert opinion. The results of the spatial association analyses quantitatively indicated that the known geothermal occurrences are strongly spatially associated with geological features such as volcanoes, craters, NNW-, NNE-, NE-direction faults and geochemical features such as hotsprings, hydrothermal alteration zones and fumaroles. Geophysical data contains temperature gradients over 100 °C/km and heat flow over $100\,mW/m^2$. In general, geochemical and geophysical data were better evidence layers than geological data for exploring geothermal resources. The spatial analyses of the case study area suggested that quantitative knowledge from hydrothermal geothermal resources was significantly useful for further exploration and for geothermal potential mapping in the case study region. The results can also be extended to the regions with nearly similar characteristics.

14/02174 Stable isotopes of hydrothermal minerals as tracers for geothermal fluids in Iceland

Pope, E. C. *et al. Geothermics*, 2014, 49, 99–110.

The Reykjanes and Krafla geothermal systems, located within the active rift zone of Iceland, are both potential venues for exploitation of deep supercritical fluids by the Iceland Deep Drilling Project. An essential aspect of properly characterizing geochemical and hydrologic processes occurring at supercritical depths is establishing the source, composition and evolution of geothermal fluids. Traditionally, hydrogen isotopes of thermal fluids are used to determine their source. The study shows that for these, and likely many other Icelandic geothermal systems, analysing fluid *dD* is not sufficient alone. Rather, $d^{18}O$ and *dD* of hydrothermal minerals in conjunction with geochemical characteristics of extant geothermal fluids are necessary to characterize the source and geologic evolution of geothermal reservoir fluids. The authors review results from existing drill holes in the Reykjanes and Krafla geothermal systems to depths of 3 km, and explore the utility of using stable isotopes in alteration minerals such as epidote to assess the hydrogeology of extinct volcano-hydrothermal systems by presenting new data from the Geitafell fossil hydrothermal system in south-east Iceland.

14/02175 Sustainability and policy for the thermal use of shallow geothermal energy

Hähnlein, S. *et al. Energy Policy*, 2013, 59, 914–925.

Shallow geothermal energy is a renewable energy resource that has become increasingly important. However, the use has environmental, technical and social consequences. Biological, chemical and physical characteristics of groundwater and subsurface are influenced by the development of this resource. To guarantee a sustainable use it is therefore necessary to consider environmental and technical criteria, such as changes in groundwater quality and temperature. In the current study a comprehensive overview of consequences of geothermal systems in shallow aquifers is provided. It was concluded that there is still a lack of knowledge on long-term environmental consequences. Due to local differences in geology and hydrogeology as well as in technical requirements, it is not recommended that only static regulations, such as fixed and absolute temperature thresholds, are defined. Flexible temperature limits for heating and cooling the groundwater and subsurface are therefore advisable. The limits should be oriented on previously undisturbed temperatures, and chemical, physical and biological conditions of aquifers. Based on these findings, recommendations for a sustainable policy for shallow geothermal systems are provided including a potential legal framework for a sustainable use.

14/02176 The application of the parametric analysis for improved energy design of a ground source heat pump for residential buildings

Molinari, M. *et al. Energy and Buildings*, 2013, 63, 119–128.

Energy use in buildings represents a major share of the overall energy used in developed countries. The reduction of the energy demand and the efficient energy use are often seen as feasible ways for a more sustainable energy use in the built environment. Ground source heat pumps (GSHPs) are efficient systems to supply heating and cooling energy to buildings but their design is critical for their performance. Furthermore, their performance depends on the cooling and heating demand and on the environmental conditions. The need for the end-use energy for a building supplied with GSHP has been studied with regard to four parameters in two different locations. The effect of two building performance parameters, roof and external walls insulation, and of two parameters affecting the performance of GSHP, boreholes spacing and number of boreholes, have been investigated by means of factorial analysis. The results show that from an energy point of view the optimal configurations of the boreholes change depending on the variation of building parameters such as insulation. The methodology proposed allows to quantify the impact of different design configurations on the need for end-use energy.

14/02177 Thermal modelling of large scale exploitation of ground source energy in urban aquifers as a resource management tool

Herbert, A. *et al. Applied Energy*, 2013, 109, 94–103.

As part of its legal commitment to reducing CO_2 emissions, the UK has outlined a roadmap for significant increases in the use of ground source heat pumps for heating and cooling buildings. The technology is particularly suitable in new buildings, and in large commercial buildings. Such development is focused in urban areas of economic growth. This paper presents an aquifer scale model of the impact of the expansion of open loop ground source energy schemes deployed in London. The model predicts the impact for currently operating schemes, and also the potential impact of all open loop schemes that have been licensed in central London. It is concluded that there will be thermal interference between these schemes and that in areas with such a high density of ground source energy schemes, the resulting loss of efficiency will mark an effective limit to the energy available for unbalanced ground source cooling. The current unregulated approach to managing the energy resource of the chalk aquifer beneath London will not be able to sustain the demands implied by the UK roadmap for ground source energy. A more actively managed approach is needed if these energy demands are to be met, economically, in London and other centres of economic growth.

Solar energy

14/02178 A comparison between BNN and regression polynomial methods for the evaluation of the effect of soiling in large scale photovoltaic plants

Pavan, A. M. *et al. Applied Energy*, 2013, 108, 392–401.

This paper presents a comparison between two different techniques for the determination of the effect of soiling on large-scale photovoltaic plants. Four Bayesian neural network (BNN) models have been developed in order to calculate the performance at standard test conditions (STCs) of two plants installed in southern Italy before and after a complete clean-up of their modules. The differences between the STC power before and after the clean-up represent the losses due to the soiling effect. The results obtained with the BNN models are compared with the ones calculated with a well-known regression model. Although the soiling effect can have a significant impact on the photovoltaic system performance and specific models developed are applicable only to the specific location in which the testing was conducted, this study is of great importance because it suggests a procedure to be used in order to give the necessary confidence to operation and maintenance personnel in applying the right schedule of clean-ups by making the right compromise between washing cost and losses in energy production.

14/02179 A system dynamics approach for the photovoltaic energy market in Spain

Movilla, S. *et al. Energy Policy*, 2013, 60, 142–154.

This paper considers the behaviour of the photovoltaic (PV) sector in Spain and its expectations under possible scenarios. Currently, PV solar energy is not a profitable sector by itself. Therefore, the Spanish government, like the governments of other countries, has stimulated investment with subsidies. The spectacular increase of PV facilities exceeded all forecasts and the government decided to curb the trend. The present hypothesis is that continuing with this support to PV energy, the technological advances and the economy generated from the production of panels would be able to make the sector profitable in the future without the necessity of subventions. Based on this hypothesis, a computer simulation model was built using the system dynamics methodology. To test its utility, the model was challenged to fit the historical data and to explore several futures over the next few years. The model allows an understanding of the sector's behaviour under the latest policies of the Spanish government, thus helping to design future public policies. The simulation results are different depending on the adopted policy and the scenario. Therefore, these factors will determine the success or failure of the investments in this type of energy.

14/02180 Cell-BMS validation with a hardware-in-the-loop simulation of lithium-ion battery cells for electric vehicles

Dai, H. *et al. International Journal of Electrical Power & Energy Systems*, 2013, 52, 174–184.

The battery management system (BMS) plays a critical role in the development of hybrid electric vehicles, plug-in hybrid vehicles and battery electric vehicles. The cell-BMS is the lower-level part of the BMS, which generally takes care of the individual cells directly, with functions mainly including voltage detection and cell balancing. In this paper, a configurable battery cell emulating system is developed to implement the hardware-in-the-loop (HIL) validation of the cell-BMS. The battery cell dynamics is simulated with a parameter-configurable equivalent circuit model consisting of three resistors, two capacitors and a SOC-controlled voltage source. The HIL system emulates battery cell dynamics to validate the function of voltage monitoring. With the bi-directional and power-amplified outputs, the system can also evaluate the performance of both active and passive cell balancing module. Meanwhile the emulated cells can be connected in series, and can be adapted to simulate some faults, e.g. over-charge and over-discharge as well. Initial testing cases using a cell-BMS prototype for the $LiMnO_2$ based battery cells show a good performance of the system. The system standardizes function validation of the cell-BMS before the design finalization and thereby accelerates the BMS development and reduces the development costs.

14/02181 Comparison of large scale coating techniques for organic and hybrid films in polymer based solar cells

Wengeler, L. *et al. Chemical Engineering and Processing: Process Intensification*, 2013, 68, 38–44.

Polymer-based solar cells (PSC) can be manufactured in a continuous roll to roll process as a low-cost regenerative energy source. Coating ink properties and film thicknesses of 30–200 nm are challenging with respect to the manufacturing process, which itself has an important impact on film properties and cell efficiencies. This study compares the large area coating methods: knife coating, slot-die coating, and spray coating with laboratory spin coating. Properties of coating inks and a viscosity model for commercial PEDOT : PSS types are discussed. The significantly smaller viscosity to surface tension ratio, of typical coating inks for PSC compared to conventional coating inks, causes a different behaviour during the coating process. Wet film thickness, homogeneity, and process stability and their dependence on process parameters are addressed for each coating method. Hole-conductive and photoactive layers, consisting of polymer-fullerene and polymer-nanoparticle blends, are then compared with respect to homogeneity, atomic force microscopy topography and absorption spectra. First results indicate that the coating method itself has an impact on polymer-fullerene film morphology and opto-electric properties.

14/02182 Determination of thermal performance calculation of two different types solar air collectors with the use of artificial neural networks

Benli, H. *International Journal of Heat and Mass Transfer*, 2013, 60, 1–7.

In this study, two different surface shaped solar air collectors are constructed and examined experimentally; corrugated and trapeze shaped. Experiments are carried out between 09.00 and 17.00 in October under the prevailing weather conditions of Elaziğ, Turkey. Thermal performances belonging to experimental systems are calculated by using data obtained from experiments. A feed-forward neural network based on back propagation algorithm was developed to predict thermal performances of solar air collectors. The measured data and calculated performance values are used following the Levenberg–Marquardt design. Calculated values of thermal performances are compared to predicted values. It is concluded that an artificial neural network can be used for the prediction of thermal performances of solar air collectors as an accurate method in this system.

14/02183 Energy and sizing analyses of parabolic trough solar collector integrated with steam and binary vapor cycles

Al-Sulaiman, F. A. *Energy*, 2013, 58, 561–570.

In this study, solar field sizing and overall performance of different vapour cycles are examined. The systems considered are parabolic trough solar collectors integrated with either a binary vapour cycle or a steam Rankine cycle (SRC). The binary vapour cycle consists of an SRC as a topping cycle and an organic Rankine cycle as a bottoming cycle. Seven refrigerants are examined for the bottoming cycle: R600, R600a, R134a, R152a, R290, R407c and ammonia. This study reveals that significant reduction in the solar field size is gained due to the performance improvement when the binary vapour cycle is considered as compared to a SRC with atmospheric condensing pressure; however, SRC with vacuum pressure has the best performance and smallest solar field size. It further reveals that the R134a binary vapour cycle has the best performance among the binary vapour cycles considered and, thus, requires the smallest solar field size while the R600a binary vapour cycle has the lowest performance. Finally, optimization shows that lowering the mass flow rate of the heat transfer fluid per each solar collector row, within the range considered, results in a reduction of the required number of solar collector rows and, thus, in savings.

14/02184 First results of incentives policy on grid interconnected photovoltaic systems development in Greece

Tsilingiridis, G. and Ikonomopoulos, A. *Energy Policy*, 2013, 58, 303–311.

The present study provides insights into how the national legislation affected the development of connected to the grid photovoltaic (PV) systems in Greece from January 2007 to June 2012. It analyses the evolution of PV systems installed capacity in Greece, compared to the targets set, as well as the PV electricity production and CO_2 emissions reduction. Moreover the geographical and the size distribution of installed capacity are examined. Up to June 2012, more than 820 MW_p had been installed, covering 55% of the 2014 national PV target capacity of 1500 MW_p. The majority of installed and licensed PV systems is in the class of 20–150 kW_p, while the share of PV systems larger than 150 kW_p is increasing steadily. The majority of installed capacity is located in southern Greece regions, where the solar potential is higher, with Peloponnesus having 15.4% of the total. The total licensed PV capacity, which is more than 2.400 MW_p exceeding not only the national 2014 target but also the 2020 target of 2200 MW_p for PV plants, together with the accelerated construction rate, which during 2012 is 49 MW_p per month, allow the save prediction that the 2014 target will be overcome.

14/02185 Low and medium temperature solar thermal collector based in innovative materials and improved heat exchange performance

Fernández, A. and Dieste, J. A. *Energy Conversion and Management*, 2013, 75, 118–129.

A low and medium temperature solar thermal collector for economical supply of heat between 40 and 90 °C has been developed. It is based on solar concentrating systems, heat transfer optimization and substitution of metallic materials by plastic ones. The basic concept is the integration of a flat absorber strip inside semi-circular reflector channels in contact with heated water without pressurization. This collector is intended to be more efficient and cheaper than what actual commercial collectors usually are so that the access to a clean and renewable energy would be more quickly redeemable and its use more effective during its life cycle, expanding its common application range. The substitution of traditional materials by surface-treated aluminium with $TiNO_x$ for the absorber and chromed thermoformed ABS for the reflector simplifies the production and assembly process. The definitive prototype has an aperture area of 0.225 m^2. It was tested in Zaragoza, Spain, and the accumulated efficiency was between 41% and 57%, and the instantaneous efficiency reached 98% depending on the weather conditions. As all trials were made in parallel with a commercial collector, in several cases the performance was over the commercial one.

14/02186 Maximum power point tracking on stand-alone solar power system: three-point-weighting method incorporating mid-point tracking

Wu, Y.-C. *et al. International Journal of Electrical Power & Energy Systems*, 2013, 52, 14–24.

This paper proposes a three-point-weighting method that incorporates mid-point tracking to improve the drawback of the perturbation and observation method and to enhance the efficiency of the three-point-weighting method. A design was simulated with PSIM, followed by hardware tests of a stand-alone solar power system using real-time Matlab/Simulink hardware-in-the-loop, for observing the efficiency of the perturbation and observation method, the three-point-weighting method, and the proposed method. It was found that the proposed method tracked better than the three-point-weighting method, and it was capable of improving the deficiency of perturbation and observation method that has difficulty to track from the open-circuit voltage (on the right-hand side of the *P–V* curve) as well as enhancing the precision of the three-point-weighting method in the case of zero-weight.

14/02187 Modeling of the rock bed thermal energy storage system of a combined cycle solar thermal power plant in South Africa

Heller, L. and Gauché, P. *Solar Energy*, 2013, 93, 345–356.

A thermocline-based rock bed thermal energy storage system potentially offers a cheap and simple way of achieving dispatchability in an air-cooled central receiver concentrating solar power (CSP) plants. In order to efficiently match heliostat field size, storage dimensions, back-up fuel consumption and turbine sizes for non-stop power generation and economic feasibility, year-long power plant simulations have to be run. This paper focuses on the storage as the centre of incoming and outgoing thermal energy. The derived storage model has one spatial dimension which is justified by the high tube-to-particle diameter ratio and because yearly aggregated – and not momentary – values are of interest. A validation of the correlations with data from the literature shows acceptable agreement. Sensitivity analyses indicate that, due to low costs of the storage system, above certain minimum storage dimensions, the influence on energetic and monetary performance indicators is marginal. The calculated LCOE is in the range of €0.11–0.18/kW h and in agreement with other studies on combined cycle CSP.

14/02188 Numerical simulation of wind flow around a parabolic trough solar collector

Hachicha, A. A. *et al. Applied Energy*, 2013, 107, 426–437.

The use of parabolic trough solar technology in solar power plants has been increased in recent years. Such devices are located in open terrain and can be the subject of strong winds. As a result, the stability of these devices to track accurately the sun and the convection heat transfer from the receiver tube could be affected. In this paper, a detailed numerical aerodynamic and heat transfer model based on large eddy simulations modelling for this equipment is presented. First, the model is verified on a circular cylinder in a cross-flow. The drag forces and the heat transfer coefficients are then validated with available experimental measurements. After that, simulations are performed on an Eurotrough solar collector to study the fluid flow and heat transfer around the solar collector and its receiver. Computations are carried out for a Reynolds number of $Re_W = 3.6 \times 10^5$ (based on the aperture) and for various pitch angles ($\theta = 0°$, 45°, 90°, 135°, 180°, 270°). The aerodynamic coefficients are calculated around the solar collector and validated with measurements performed in wind tunnel tests. Instantaneous velocity field is also studied and compared to aerodynamic coefficients for different pitch angles. The time-averaged flow is characterized by the formation of several recirculation regions around the solar collector and the receiver tube depending on the pitch angle. The study also presents a comparative study of the heat transfer coefficients around the heat collector element with the circular cylinder in a cross-flow and the effect of the pitch angle on the Nusselt number.

14/02189 Performance assessment of different solar photovoltaic technologies under similar outdoor conditions

Sharma, V. *et al. Energy*, 2013, 58, 511–518.

The site-specific evaluation of a solar photovoltaic technology helps in identifying its suitability for that location. The objective of this study was to assess the suitability of different photovoltaic technologies under Indian climatic conditions. The performance assessment of photovoltaic technology arrays consisting of polycrystalline silicon, hetero-junction with intrinsic thin layer silicon and amorphous single junction silicon was carried out at a test facility in the Solar Energy Centre of India. The energy yield and performance ratio of each technology were evaluated. The performance of each technology was also predicted using photovoltaic system simulation software and compared with the measured performance. A correction to the module efficiency, resulted in reducing the absolute percentage error between measured and predicted annual energy yield and performance ratio values to 4.89%, 4.94%, 1.16% and 4.34%, 4.93%, 1.88% for p-Si, HIT and a-Si arrays, respectively. The performance comparison showed that HIT and a-Si arrays have performed better than p-Si array at this location. The energy yield of a-Si modules was found to be 14% more in summer months and 6% less in winter months in comparison to p-Si modules. The HIT modules were found to produce 4–12% more energy consistently than p-Si modules.

14/02190 Phase-change materials to improve solar panel's performance

Biwole, P. H. *et al. Energy and Buildings*, 2013, 62, 59–67.

High operating temperatures induce a loss of efficiency in solar photovoltaic and thermal panels. This paper investigates the use of phase-change materials (PCM) to maintain the temperature of the panels close to ambient. The main focus of the study is the computational fluid dynamics modelling of heat and mass transfers in a system composed of an impure phase change material situated in the back of a solar panel. A variation of the enthalpy method allows simulating the thermo-physical change of the material properties. The buoyancy term in Navier–Stokes' momentum conservation equation is modified through an additional term which forces the velocity field to be non-existent when the PCM is solid. For validation purposes, isotherms and velocity fields are calculated and compared to those from an experimental set-up. Results show that adding a PCM on the back of a solar panel can maintain the panel's operating temperature under 40 °C for 80 min under a constant solar radiation of 1000 W/m^2.

14/02191 Photovoltaics in agriculture: a case study on decision making of farmers

Brudermann, T. *et al. Energy Policy*, 2013, 61, 96–103.

This paper aims to identify the success factors, incentives, barriers and challenges in the adoption process of photovoltaics (PV) in the agricultural sector, with particular focus placed on decision making of individual farmers and network effects. The authors investigated a successful case of an Austrian farmers' association that set up a community power plant concept and a society for facilitating PV adoption among farmers. It was found that PV adoption decisions are driven by economic and environmental considerations and that while ethical considerations are relatively strong among farmers, they cannot be used as predictors in the decision making process. Results furthermore suggest that while adoption of PV increases belief in technological progress as a solution to environmental problems, it may simultaneously lead to a weakening in the belief that underlying lifestyle changes are necessary. The conclusions address crucial aspects of PV adoption in agriculture, and implications for policy measures related to respective community initiatives.

14/02192 Porosity control in thin film solar cells

Huang, J. *et al. Chemical Engineering Science*, 2013, 94, 44–53.

This work focuses on the simulation and control of a porous silicon deposition process used in the manufacture of thin film solar cell systems. Initially, a thin film deposition process is simulated via a kinetic Monte Carlo (kMC) method on a triangular lattice following the model developed in an earlier study. Then a closed-form differential equation model is introduced to predict the dynamics of the kMC model and the parameters in this model are identified by fitting to open-loop kMC simulation results. A model predictive controller (MPC) is also designed and implemented on the kMC model. Extensive closed-loop simulation results demonstrate that both film thickness and porosity can be regulated to desired values. Finally, the porosity control framework is extended into a two-stage dual porosity deposition process, with two different porosity set-points for each stage. The closed-loop results demonstrate that at the end of both stages the film porosity values can be successfully regulated at the requested set-point values.

14/02193 Simple and low-cost method of planning for tree growth and lifetime effects on solar photovoltaic systems performance

Dereli, Z. *et al. Solar Energy*, 2013, 95, 300–307.

The use of distributed solar photovoltaic (PV) systems is growing more common as solar energy conversion efficiencies increase while costs decrease. Thus, PV system installations are increasing in non-optimal locations such as those potentially shaded with trees. Tree-related shading can cause a significant power loss and an increasing collection of laws have been enacted and are under development to protect the right of PV owners to solar access. This paper provides a new method to predict the shading losses for a given tree species, orientation to a PV array, and geographic location using existing free tools in order to assist in the prevention of conflicts by creating an environment where PV systems and trees can coexist while maximizing PV performance. This methodology is applied to a case study in the Midwest USA. Tree growth characteristics including height, crown width, and growth rate were investigated. Minimum planting distances were quantified based on tree species and orientation of planting with respect to the PV system and conclusions were drawn from the results. This novel open low-cost method to predict and prevent tree shading from negatively impacting the performance of roof-mounted PV systems assists in planning of technical design.

14/02194 Simulation and an experimental investigation of SVPWM technique on a multilevel voltage source inverter for photovoltaic systems

Rajkumar, M. V. *et al. International Journal of Electrical Power & Energy Systems*, 2013, 52, 116–131.

This paper presents a space vector pulse width modulation (SVPWM) control for a three-phase five-level diode clamped multilevel inverter (DCMLI) for photovoltaic (PV) systems. SVPWM algorithm uses a simple mapping to generate gate signals for the inverter. The location of the reference vector and time are easily determined. The maximum power point tracking (MPPT) is capable of extracting maximum power from PV array connected to each DC link voltage level. The MPPT algorithm is solved by fuzzy logic controller. A digital design of a generator SVPWM using hardware description language (VHDL) is proposed and implemented on a field programmable gate array (FPGA). This is done to achieve high dynamic performance with low total harmonic distortion (THD). Simulation and experimental results are given to verify the implemented SVPWM control in terms of THD. The results are compared with conventional sinusoidal pulse width modulation (SPWM) in terms of lower THD is obtained. Finally, the implementation on a FPGA is tested in a laboratory with a real prototype using a three-level three-phase voltage source inverter. Experimental results are presented to verify the effectiveness and accuracy of the proposed system. This scheme can be easily extended to an n-level inverter for PV system.

14/02195 Simulation of thermocline storage for solar thermal power plants: from dimensionless results to prototypes and real-size tanks

Bayón, R. and Rojas, E. *International Journal of Heat and Mass Transfer*, 2013, 60, 713–721.

A single-phase one-dimensional model called CIEMAT1D1SF has been developed for characterizing the behaviour of thermocline tanks with an effective storage medium formed by either a liquid or a liquid and a packed-bed. Despite its simplicity, this model has been validated with experimental data and the results of tank performance are similar to those obtained by other authors using more complex simulation models. In order to obtain general results the thermal equation has been non-dimensionalized and the resulting expression only depends on the parameter called dimensionless velocity, v^*. It has been observed that thermocline thickness decreases as v^* increases attaining a minimum value when $v^* \geq 2350$ while tank efficiency increases with v^* up to a maximum of about 87% also for $v^* \geq 2350$. From these results the design equation for building thermocline storage tanks with maximum theoretical efficiency has been established. Since this design equation depends on tank dimensions and thermal power, small thermocline tanks and hence prototypes are not expected to behave in the same way as large or real-size tanks. Therefore maximum efficiency guideline plots for thermocline tanks with different storage media have been presented for various temperature intervals. In these plots thermal power has proven to be the critical design parameter because the larger the power the higher the degree of freedom for choosing tank dimensions and hence storage capacity and charging/discharging time. Therefore, the use of these guideline plots in the design process of thermocline prototypes are strongly recommended.

14/02196 Soiling losses for solar photovoltaic systems in California

Mejia, F. A. and Kleissl, J. *Solar Energy*, 2013, 95, 357–363.

Soiling is the accumulation of dust on solar panels that causes a decrease in the solar photovoltaic (PV) system's efficiency. The changes in conversion efficiency of 186 residential and commercial PV sites were quantified during dry periods over the course of 2010 with respect to rain events observed at nearby weather stations and using satellite solar resource data. Soiling losses averaged 0.051% per day overall and 26% of the sites had losses greater than 0.1% per day. Sites with small tilt angles ($<5^\circ$) had larger soiling losses while differences by region were not statistically significant.

14/02197 Solar forecasting methods for renewable energy integration

Inman, R. H. *et al. Progress in Energy and Combustion Science*, 2013, 39, (6), 535–576.

The higher penetration of renewable resources in the energy portfolios of several communities accentuates the need for accurate forecasting of variable resources (solar, wind, tidal) at several different temporal scales in order to achieve power grid balance. Solar generation technologies have experienced strong energy market growth in the past few years, with corresponding increase in local grid penetration rates. As is the case with wind, the solar resource at the ground level is highly variable mostly due to cloud cover variability, atmospheric aerosol levels, and indirectly and to a lesser extent, participating gases in the atmosphere. The inherent variability of solar generation at higher grid penetration levels poses problems associated with the cost of reserves, dispatchable and ancillary generation, and grid reliability in general. As a result, high accuracy forecast systems are required for multiple time horizons that are associated with regulation, dispatching, scheduling and unit commitment. Here the authors review the theory behind these forecasting methodologies, and a number of successful applications of solar forecasting methods for both the solar resource and the power output of solar plants at the utility scale level.

14/02198 Synthesis of a graphene–tungsten composite with improved dispersibility of graphene in an ethanol solution and its use as a counter electrode for dye-sensitised solar cells

Munkhbayar, B. *et al. Journal of Power Sources*, 2013, 230, 207–217.

The paper reports a nanocomposite (graphene and tungsten, GN–W) that was successfully used as an alternative to a conventional Pt counter electrode in dye-sensitized solar cells (DSSCs). The dispersibility of the GN structure in ethanol was enhanced by acid oxidation and planetary ball milling. Raw, purified and purified and ground GN structures were spin coated onto fluorine-doped tin oxide (FTO) glass substrates and examined as catalytic films on the counter electrodes of DSSCs. Purified and ground GNs exhibited the best photovoltaic performance (4.55%) among these structures. The grinding method was found effective for upgrading the dispersibility of GNs in a base fluid and the photovoltaic efficiency results. Based on the photovoltaic efficiency results of the DSSCs with different GN structures, the purified and ground GN structure was selected and incorporated with tungsten. A composite film of GN–W was used as a catalytic film on the counter electrode of a DSSC. The DSSC fabricated with the GN–W composite counter electrode achieved a photovoltaic efficiency of 5.88%. This performance is comparable to that of a DSSC with a standard Pt counter electrode (5.92%).

14/02199 The application of soft computing methods for MPPT of PV system: a technological and status review

Salam, Z. *et al. Applied Energy*, 2013, 107, 135–148.

With the availability of powerful and low-cost computing power, maximum power point tracking (MPPT) that utilizes soft computing (SC) techniques are attracting substantial interests from the PV communities. Due to their flexibility and ability to handle non-linear problems, robust SC-based MPPT schemes can be developed. Furthermore, the adaptive in nature SC algorithms is suitable in handling adverse environmental conditions such as partial shading and rapid changes in irradiance. To date, there are several works on MPPT using SC, from these approximately 45 published works directly related to MPPT were selected. However, information on these methods are scattered and there appears to be an absence for a comprehensive review paper on this topic. This work summarizes the current technology and status of SC MPPT as reported in various literature. It also provides an evaluation on the performance of various SC methods based on several criteria, namely PV array dependency, convergence time, ability to handle partial shading conditions, algorithm complexity and hardware/practical implementation. It is envisaged that the information gathered in this paper will be a valuable one-stop source of information for researchers, as well as providing a direction for future research in this area.

14/02200 The solar photovoltaic feed-in tariff scheme in New South Wales, Australia

Martin, N. and Rice, J. *Energy Policy*, 2013, 61, 697–706.

Solar photovoltaic (PV) electricity systems are part of Australia's energy supply matrix. In the case of New South Wales (NSW), the state government has had to deal with a complex policy problem. In order to play its role in the federal small-scale renewable energy scheme, the NSW government initiated the 7-year solar bonus scheme in 2010. However, in attempting to maximize community investment in small-scale solar PV systems, it relied on faulty financial modelling that applied a generous feed-in tariff (FiT) and underestimated the level of investor participation and installed capacity. Consequently, the scheme has resulted in very high public costs that will require policy changes that bring investors and energy retailers into conflict, and unpopular electricity retail price adjustments. This paper uses a structured case and stakeholder analysis to critically analyse the FiT policy, while also highlighting important lessons for policymakers engaging in FiT design.

14/02201 Theoretical and experimental investigation on a thermoelectric cooling and heating system driven by solar
He, W. *et al. Applied Energy*, 2013, 107, 89–97.
Buildings composited with thermoelectric cooling and heating systems use solar energy to cool rooms in summer and heat rooms in winter via thermoelectric devices and photovoltaic/thermal (PV/T) dual function modules. In summer, the thermoelectric device works as a Peltier cooler when electrical power supplied by PV/T modules is applied on it. The cold side absorbs heat from indoor to decrease the temperature of the room. In the meanwhile, the thermal energy gained both from the hot side and PV/T system is collected to heat domestic water by heat pipes. In winter, the voltage applied on thermoelectric device is reversed with PV/T modules being power and heat source simultaneously to thermoelectric device and then thermoelectric device could release heat to increase the temperature of the room. The experiments has been done in a model room whose volume is 0.125 m^3, in summer condition, using solar panel whose area is 0.5 m^2. The minimum temperature 17 °C is achieved, with COP of the thermoelectric device higher than 0.45. The temperature of water in the storage tank with a volume of 18.5 L has risen about 9 °C. The thermal efficiency of the system is 12.06%. This simple and environmentally friendly can reduce cooling and heating load in a room.

14/02202 Unsymmetric three-layer laminate with soft core for photovoltaic modules
Weps, M. *et al. Composite Structures*, 2013, 105, 332–339.
Unsymmetrical laminates are designed for the use in new lightweight construction of photovoltaic modules. One feature of the laminate is relatively thin and compliant polymeric core layer for embedding solar cells. To assess mechanical properties of the core a three-layer beam is proposed as a model structure. For the structural analysis a layer-wise beam theory is developed. Robust relationships between the maximum deflection, the transverse shear strain of the core layer and the applied force in a three-point-bending test of laminated beam samples are derived. Furthermore, a three-dimensional finite element analysis is performed to verify the assumptions of the beam theory. Three-point-bending tests for laminated beams are performed. The experimentally obtained load–deflection curves are compared with the theoretical results.

14/02203 Urban solar energy potential in Greece: a statistical calculation model of suitable built roof areas for photovoltaics
Karteris, M. *et al. Energy and Buildings*, 2013, 62, 459–468.
Determining the actual solar potential for applications in the complex urban environment is a difficult task, particularly when there is a lack in background information, such as the texture and structure of the urban landscape, as this was until very recently the case in Greece. In this paper a simplified yet effective methodological approach for the evaluation of solar architecturally suitable areas of flat roof surfaces on typical multi-storey, multifamily buildings is presented. It is based on a statistical calculation model for solar potential that has been validated, by analysing actual measurements carried out in the city of Thessaloniki in northern Greece. The model can be either used by private engineers or it can be alternatively incorporated in geoinformatics decision-making tools, such as GIS, to aid planners, regulators and developers to determine the solar potential. Finally, it is of great interest to notice that the photovoltaic potential of the multifamily buildings considered in the validation, proved to be rather poor. The solar utilization roof factor in the majority of the examined building cases was approximated only between 25% and 50%.

14/02204 Variations in photovoltaic performance due to climate and low-slope roof choice
Nagengast, A. *et al. Energy and Buildings*, 2013, 64, 493–502.
With urban space at a premium, roofs are being targeted as an opportunity to deploy sustainable energy technologies for buildings. This research evaluates the combination of green roofs and solar photovoltaics specifically through their temperature and electricity production relationship. Measurements over a 1-year study period from 1 July 2011 to 30 June 2012 from a large field project in Pittsburgh, Pennsylvania, USA were used to determine the differences in power output from green and black roofs as well as to derive two regression functions for back-surface panel temperature and photovoltaic (PV) output. These estimation functions were applied to three different cities (San Diego, CA; Huntsville, AL and Phoenix, AZ) chosen to represent a wide range of irradiance and temperature values. Based on the specific test-bed configuration, the green or black roof choice under the PV panels had little impact on the PV performance. The difference in magnitude of power generation for green roof–PV compared with black roof–PV assemblies was small (0.5%) corresponding to an annual loss of $9/60 panels in Pittsburgh and a benefit of approximately $8/60 panels per year in Phoenix. Results also suggest that sites consistently above 25 °C will most likely see a small, positive impact from a green roof–PV combination. Building managers and designers should consider this temperature and power output interaction a minor economic factor in roof decisions.

Wind energy

14/02205 A comparison between the ECMWF and COSMO ensemble prediction systems applied to short-term wind power forecasting on real data
Alessandrini, S. *et al. Applied Energy*, 2013, 107, 271–280.
Wind power forecasting (WPF) represents a crucial tool to reduce problems of grid integration and to facilitate energy trading. By now it is advantageous to associate a deterministic forecast with a probabilistic one, in order to give to the end-users information about prediction uncertainty together with a single forecast power value for each future time horizon. A comparison between two different ensemble forecasting models, ECMWF EPS (Ensemble Prediction System in use at the European Centre for Medium-Range Weather Forecasts) and COSMO-LEPS (Limited-area Ensemble Prediction System developed within COnsortium for Small-scale MOdelling) applied for power forecasts on a real case in Southern Italy is presented. The approach is based on retrieving meteorological ensemble variables (i.e. wind speed, wind direction), using them to create a power probability density function for each 0–72 h ahead forecast horizon. A statistical calibration of the ensemble wind speed members based on the use of past wind speed measurements is explained. The two models are compared using common verification indices and diagrams. The higher horizontal resolution model (COSMO-LEPS) shows slightly better performances, especially for lead times from 27 to 48 h ahead. For longer lead times the increase in resolution does not seem crucial to obtain better results. A deterministic application using the mean of each ensemble system is also presented and compared with a higher resolution 0–72 h ahead power forecast based on the ECMWF deterministic model. It is noticeable that, in a deterministic approach, a higher resolution of the ensemble system can lead to slightly better results that are comparable with those of the high resolution deterministic model.

14/02206 An experimental investigation into the influence of unsteady wind on the performance of a vertical axis wind turbine
Danao, L. A. *et al. Applied Energy*, 2013, 107, 403–411.
An experimental investigation was carried out on a wind tunnel scale vertical axis wind turbine with unsteady wind conditions. The wind speed at which testing was conducted was 7 m/s (giving a Reynolds number of around 50,000) with both 7% and 12% fluctuations in wind velocity at a frequency of 0.5 Hz. Rotational speed fluctuations in the VAWT were induced by the unsteady wind and these were used to derive instantaneous turbine rotor power. The results show the unsteady power coefficient (CP) fluctuates following the changes in wind speed. The time average of the unsteady CP with a 7% fluctuation in wind velocity was very close to that with steady wind conditions while 12% fluctuations in wind speed resulted in a drop in the mean CP, meaning unsteady winds of such amplitudes are detrimental to the energy yields from these wind turbines. At mean rotational speeds corresponding to tip speed ratios (λ) beyond peak CP, no significant hysteresis was observed for both 7% and 12% fluctuations. However, substantial hysteresis is seen for conditions where mean λ is below peak CP.

14/02207 Combined Monte Carlo simulation and OPF for wind turbines integration into distribution networks
Mokryani, G. and Siano, P. *Electric Power Systems Research*, 2013, 103, 37–48.
In this paper, a probabilistic method to evaluate the impact of wind turbines (WTs) integration into distribution systems within a market environment is proposed. Combined Monte Carlo simulation (MCS)

technique and market-based optimal power flow (OPF) are used to maximize the social welfare considering different combinations of wind generation and load demand over a year. MCS is used to model the uncertainties related to the stochastic nature of wind and the volatility of WTs' offers. The market-based OPF is solved by using step-controlled primal dual interior point method considering network constraints. The method is conceived for distribution network operators (DNOs) in order to evaluate the effect of WTs integration into the grid. The effectiveness of the proposed method is demonstrated with an 84-bus 11.4 kV radial distribution system.

14/02208 Comparative study on fault responses of synchronous generators and wind turbine generators using transient stability index based on transient energy function
Chowdhury, M. A. *et al. International Journal of Electrical Power & Energy Systems*, 2013, 51, 145–152.
Increasing wind power penetration into the grid justifies the requirement of the analysis of wind power dynamics, especially during transient faults. Quantitative transient stability (TS) assessment is required to provide deeper insight into the TS problems for speeding up the operational decision making process. This can be achieved by evaluating transient stability index (TSI) through the assessment of transient energy function. This paper carries out the quantitative insight of the impact of different generator technologies on the grid by comparatively studying the impacts of the fault clearing time, the grid coupling, the inertia constant, the generator terminal voltage sag and the slip on fault responses with the TSI between synchronous generators and wind turbine generators, such as squirrel cage induction generators and doubly fed induction generators.

14/02209 Recurrent modified Elman neural network control of PM synchronous generator system using wind turbine emulator of PM synchronous servo motor drive
Lin, C.-H. *International Journal of Electrical Power & Energy Systems*, 2013, 52, 143–160.
The recurrent modified Elman neural network (NN) controlled a permanent magnet (PM) synchronous generator system, which is driven by wind turbine emulator of a PM synchronous motor servo drive, is developed to regulate output voltage of rectifier (or AC to DC power converter) and inverter (or DC to AC power converter) in this study. First, the wind turbine emulator of a closed loop PM synchronous motor servo drive is designed to produce the maximum power for the PM synchronous generator system. Then, the rotor speed of the PM synchronous generator, the output DC bus voltage and current of the rectifier are detected simultaneously to yield maximum power output of the rectifier through DC bus power control. Because the PM synchronous generator system is a non-linear and time-varying dynamic system, the online training recurrent modified Elman NN control system is developed to regulate DC bus voltage of the rectifier and AC line voltage of the inverter in order to improve the control performance. Furthermore, the online training recurrent modified Elman NN control system with the variable learning rate is derived based on Lyapunov stability theorem, so that the stability of the system can be guaranteed. Finally, some experimental results are verified to show the effectiveness of the proposed recurrent modified Elman NN controlled PM synchronous generator system.

14/02210 Statistical analysis of installed wind capacity in the United States
Staid, A. and Guikema, S. D. *Energy Policy*, 2013, 60, 378–385.
There is a large disparity in the amount of wind power capacity installed in each of the states in the USA. It is often thought that the different policies of individual state governments are the main reason for these differences, but this may not necessarily be the case. The aim of this paper is to use statistical methods to study the factors that have the most influence on the amount of installed wind capacity in each state. From this analysis, the authors were able to use these variables to accurately predict the installed wind capacity and to gain insight into the driving factors for wind power development and the reasons behind the differences among states. Using their best model, the authors found that the most important variables for explaining the amount of wind capacity have to do with the physical and geographic characteristics of the state as opposed to policies in place that favour renewable energy.

14/02211 The role of values in public beliefs and attitudes towards commercial wind energy
Bidwell, D. *Energy Policy*, 2013, 58, 189–199.
Mandates for renewable energy lead to siting disputes, because meeting the mandates requires the development of renewable energy production facilities. Proposals for one common form of renewable energy, commercial wind farms, are frequently met with forceful local opposition. Dissatisfied with simplistic explanations for this opposition (i.e. 'not-in-my-backyard'), social scientists have urged a more nuanced understanding of public attitudes towards wind energy and other renewables. Based on a survey of residents of coastal Michigan, this article explores the role of general values and beliefs in shaping attitudes towards the potential development of commercial wind energy projects in or near respondents' communities. Structural equation modelling reveals that support of commercial wind energy depends largely on a belief that wind farms will provide economic benefits to the community. Underlying values have substantial and important indirect effects on beliefs regarding the likely economic outcomes of wind farm development. Altruistic values buoy wind energy attitudes, while values of traditionalism diminish wind energy support. The pivotal role of values in attitudes towards renewables lends support for more participatory development processes.

Others, including economics

14/02212 A comprehensive economical and environmental analysis of the renewable power generating systems for Kirklareli University, Turkey
Gokcol, C. and Dursun, B. *Energy and Buildings*, 2013, 64, 249–257.
This paper is to investigate various renewable based hybrid systems with five minimum renewable penetration rates (RPR) for Pinarhisar Educational campus in Kirklareli University, Turkey, to present the effects of making the system more sensitive to the environment on the total net present cost (NPC) and cost of energy (COE) and also to search for the optimum configuration of the hybrid systems. Yearly wind and solar data are considered in this study. Optimal stand-alone and grid connected hybrid systems with different minimum RPRs, are determined and analysed in detail by using HOMER software and compared among themselves considering COE, total NPC, emission rates. Additionally, sensitivity analysis is performed to determine the cost of generating the cleaner energy from the hybrid systems. As a result, it can be highlighted that gradual increases in the total NPC and COE occur in the region where RPRs are between 0 and 70%, and that there are dramatic increases in both the total NPC and COE for the RPRs above 70%. Moreover, emission rates for CO_2, SO_2 and NO_x basically decrease as RPR increases from 0% to 90% and they decrease linearly until RPR is 80% while they are nearly zero for the values more than 80%.

14/02213 A hybrid tool to combine multi-objective optimization and multi-criterion decision making in designing standalone hybrid energy systems
Perera, A. T. D. *et al. Applied Energy*, 2013, 107, 412–425.
Hybrid energy systems (HESs) are becoming popular for standalone applications due to global concern regarding greenhouse gas (GHG) emissions and depletion of fossil fuel resources. Research in the optimal design of HESs is ongoing, with numerous optimization techniques giving special emphasis to Pareto optimization, incorporating conflicting objectives. The subsequent decision-making process including the non-dominant set of solutions has yet to be addressed. This work focuses on combining multi-objective optimization with a multi-criterion decision-making (MCDM) technique to support decision makers in the process of designing HESs. Four different objectives, i.e. levelized energy cost (LEC), unmet load fraction, wasted renewable energy (WRE) and fuel consumption are used to obtain the Pareto front. A decision support tool based on fuzzy TOPSIS and level diagrams is proposed to analyse the Pareto front and support the subsequent decision-making activity. A case study is used to illustrate the applicability of the proposed method. The study shows that the novel method is useful when determining the relative weights of objectives, providing a detailed picture of the objective space to the designer when coming up with the optimum system. The technique proposed in this study can be further extended to analyse similar problems in energy system design where MCDM is necessary after multi-objective optimization.

14/02214 Civilized swarm optimization for multiobjective short-term hydrothermal scheduling
Selvakumar, A. I. *International Journal of Electrical Power & Energy Systems*, 2013, 51, 178–189.
This paper presents a solution technique for multiobjective short-term hydrothermal scheduling (MSTHTS) through civilized swarm optimization (CSO) which is the hybrid of society–civilization algorithm (SCA) and particle swarm optimization (PSO). The intra-and inter-society communication mechanisms of SCA have been embedded into the food-searching strategy of PSO to form CSO. The MSTHTS problem is formulated by considering economic and emission objectives. A new ideal guide method has been proposed to find out the Pareto-optimal front. Multi-reservoir cascaded hydro power plants having non-linear generation characteristics and thermal power plants with non-smooth cost and emission curves are considered for analysis. Other aspects such as, water transport delay, water availability, storage conformity,

power loss and operating limits are fully accounted in the problem formulation. The performance of the proposed CSO is demonstrated through two MSTHTS problems and the results are compared with those presented in the literature. CSO along with the new ideal guide method outperforms all the previous approaches by providing quality Pareto-optimal fronts.

14/02215 Economic and environmental impacts of a PV powered workplace parking garage charging station

Tulpule, P. J. *et al. Applied Energy*, 2013, 108, 323–332.

Plug-in hybrid electric vehicles (PHEVs) and electric vehicles (EVs) have high potential for reducing fuel consumption and emissions, and for providing a way to utilize renewable energy sources for the transportation sector. On the other hand, charging millions of PEVs could overload the power grid, increase emissions and significantly alter economic characteristics. A day-time photovoltaic (PV) based, plug-in electric vehicle charging station located in a workplace parking garage is considered in this research. The results show the impact of PV based workplace charging on the economics and emissions from the power grid. An optimal charge scheduling strategy is compared with an uncontrolled charging case to perform the economics and emissions analysis. Two locations (Columbus, Ohio and Los Angeles, California) are selected such that the analysis includes different scenarios of yearly variation of solar radiation and finance structure. A high fidelity hourly simulation model for energy economic analysis is developed considering different types of vehicles, statistical data for driving distances, parking time, installation cost, tax rebates and incentives. An incremental parking rate for accessing the charging facility is considered for economic analysis for the garage owner and the vehicle owner. The analysis is extended to consider the impact of carbon tax implementation on the driver economics and shows the feasibility of such PV-based charging stations. Parametric analysis for different parking rates and installed capacities show (i) the feasibility of a PV-based workplace charging facility, (ii) benefits to the vehicle owner and the garage owner and (iii) the need for an optimal charging controller.

14/02216 Experimental hydrodynamic study of the Qiantang River tidal bore

Huang, J. *et al. Journal of Hydrodynamics, Ser. B*, 2013, 25, (3), 481–490.

To study the hydrodynamics of a tidal bore, a physical modelling study was carried out in a rectangular flume with considerations of the tidal bore heights, the propagation speeds, the tidal current velocities, the front steepness and the bore shapes. After the validation with the field observations, the experimental results were analysed, and it was shown that: (1) the greater initial ebb velocity or the larger initial water depth impedes the tidal bore propagation, (2) the maximum bore height appears at an initial ebb velocity in the range of 0.5–1.5 m/s, (3) when the Froude number exceeds 1.2, an undular bore appears, after it exceeds 1.3, a breaking bore occurs, and after it exceeds 1.7, the bore is broken.

14/02217 How will renewable power generation be affected by climate change? The case of a metropolitan region in northwest Germany

Wachsmuth, J. *et al. Energy*, 2013, 58, 192–201.

Energy systems that primarily use wind and solar power production require the long-term storage of electricity and fully developed transmission grids. Moreover, renewables-based energy systems may be strongly affected by climate change. This study presents two models that assess the impacts of climate change on solar and wind power generation and use these models to evaluate climate projections based on the A1B scenario for Germany's north-west metropolitan region. For these projections, the seasonal profile of solar power production is not affected despite less cloud cover during the summer, while the seasonal profile of wind power production has a more pronounced seasonal peak during the winter due to slightly increasing wind speeds. The obtained seasonal profiles to different scenarios for electricity demand were compared. For each scenario the ratio of wind and solar power generation was identified that minimizes the variance of the residual load at the monthly time scale under the premise of a full supply by wind and solar power. The results suggest that the need for long-term storage of electricity and the need for extensions of the transmission grid will on the one hand decrease but on the other hand become more volatile because of climate change impacts in the German north-west metropolitan region over the next century.

14/02218 Investment barriers and incentives for marine renewable energy in the UK: an analysis of investor preferences

Leete, S. *et al. Energy Policy*, 2013, 60, 866–875.

Deployment of marine renewable energy (MRE) in the UK is desirable in order to address climate change, meet mandatory European Union renewable energy targets and provide significant economic development opportunities, including new export markets. Public funding constraints in the UK mean that substantial investment is required from the private sector to commercialize the industry. By focusing on investor attitudes and behaviours towards wave and tidal technologies, this paper reveals significant observations from the investment community with serious implications for the future of the MRE industry. Through a series of in-depth interviews with individuals from the investment community, device developers and industry support, the research seeks to identify common barriers and incentives to investment. The paper demonstrates that although investors' attitudes are generally aligned, they do appear to have changed over time. Of the participants that had previously invested in early stage MRE device development, none were likely to do so again. It is concluded that this is a function of investors' greater understanding of the scale, and unpredictability of the costs, and the length of time required to develop these technologies. This presents a significant policy challenge for all actors interested in the commercialization of wave and tidal technologies.

14/02219 Long-term scenarios and strategies for the deployment of renewable energies in Germany

Pregger, T. *et al. Energy Policy*, 2013, 59, 350–360.

The transformation of the energy supply in Germany as described in the German federal government's 2010 'energy concept' is based on a political consensus about long-term targets for energy efficiency and renewable energies. This study aims to present a consistent scenario for this transformation process reflecting the long-term implementation of renewable energies and the possible future structure of the German energy system as a whole. Structural and economic effects of this development are derived and discussed. It summarizes results of scenario analyses done by the department of Systems Analysis and Technology Assessment of the German Aerospace Centre as part of a three-year research project for the German Federal Ministry for the Environment. The underlying study provides a detailed database reflecting a long-term roadmap for the energy system transformation in Germany. The scenarios show that the policy targets are consistent and can be achieved, if appropriate policy measures are to be implemented. The economic analysis shows the amount of investments and the strong market dynamics required for new generation technologies but also the huge economic benefits that can result from this development path in terms of fuel cost savings and lower fuel imports.

14/02220 Mini-hydro: a design approach in case of torrential rivers

Barelli, L. *et al. Energy*, 2013, 58, 695–706.

The problem of designing small run-of-river hydropower plants is critical for the cost-effectiveness of the investment. In order to maximize the economic benefits, an accurate feasibility study must be effected by considering the hydrogeological characteristics of the rivers. In this paper a different design approach regarding mini- and micro-hydro plants is presented. Specifically, the proposed methodology needs to be a helpful tool to avoid sizing errors that can occur by applying the conventional calculation methods not suitable for torrential rivers. Starting from the analysis of the flow duration curve, the developed method provides an initial value for the turbine nominal flow rate and, considering the actual daily flow rate usable by the turbine, allows the optimal size to be found. The method has been developed on the basis of particular rivers, having different runoff regimes, chosen as cases study; for these rivers it has permitted to optimize the plant and find the shorter investment payback time.

14/02221 Reconciling self-sufficiency and renewable energy targets in a hydro dominated system: the view from British Columbia

Sopinka, A. *et al. Energy Policy*, 2013, 61, 223–229.

British Columbia's energy policy is at a crossroads; the Canadian province has set a goal of electricity self-sufficiency, a 93% renewable portfolio standard and a natural gas development strategy that could increase electricity consumption by 21 TWh to 33 TWh. To ascertain British Columbia's supply position, a mathematical programming model of the physical workings of the province's hydroelectric generating system is developed, with head heights at the two dominant power stations treated as variable. Using historical water inflow and reservoir level data, the model is used to investigate whether British Columbia is capable of meeting its self-sufficiency goals under various water supply and electricity demand scenarios.

14/02222 Renewable energy integration for smart sites

Kaygusuz, A. *et al. Energy and Buildings*, 2013, 64, 456–462.

Use of distributed renewable energy sources for domestic energy consumption will increase in the near future, due to its advantages as being clean and infinite energy generation possibility. This trend allows more efficient energy consumption because of reducing transmission loses and dependence of domestic appliances to grid distribution. This study investigates potentials of a smart site concept based on domestic renewable energy generation. The study addresses site-scale inte-

gration of hybrid renewable sources and grid energies as well as investigates possible advantages of the use of hybrid renewable energy systems based on solar and wind power. A continuous energy mixing strategy is used for DC integration of hybrid renewable energy (wind + solar) and the grid energy to meet site power demand. The proposed case study demonstrates that the smart site with hybrid renewable sources considerably reduces energy dependence of the house appliances to the grid which in turn presents a feasible solution for implementation of distributed generation provision for future smart grids.

14/02223 Thermo-economic assessment of a micro CHP system fuelled by geothermal and solar energy
Tempesti, D. and Fiaschi, D. *Energy*, 2013, 58, 45–51.
A micro combined heat and power (CHP) plant operating through an organic Rankine cycle (ORC) using renewable energy is analysed. The reference system is designed to produce 50 kWe. The heat sources of the system are geothermal energy at low temperature (80–100 °C) and solar energy. The system uses a solar field composed only by evacuated solar collectors, and work is produced by a single turbine. Different working fluids (e.g. R134a, R236fa, R245fa) are considered in the analysis. The aim of this paper is to assess the cost of the proposed CHP plant and to determine the most convenient working fluid through a thermo-economic analysis. The system is sized in base of the weather data of a city in the centre of Italy in three different months (January, March, July), and the main characteristics of the system (i.e. heat exchanger surface, solar collector area) are presented. The results of the thermo-economic analysis show that R245fa allows the lowest price of electricity production and the lowest overall cost of the CHP plant.

14 FUEL SCIENCE AND TECHNOLOGY

Fundamental science, analysis, instrumentation

14/02224 A facile preparation of novel Pt-decorated Ti electrode for methanol electro-oxidation by high-energy micro-arc cladding technique
Wang, X. *et al. Journal of Power Sources*, 2013, 230, 81–88.
In this paper, a novel Pt-decorated Ti electrode was prepared by a high-energy micro-arc cladding (HEMAC) technique for methanol electro-oxidation in alkaline media. The surface structure, morphology, composition and electrocatalytic properties were investigated by thin-film X-ray diffraction, scanning electron microscopy-energy dispersive X-ray analysis and electrochemical measurements. The results show that the $Pt_{arc\text{-}dep}Ti$ surface mainly comprises Ti, Pt, Pt_3Ti and $PtTi_3$. Moreover, a coarsening topographical morphology can be obtained, being composed of numerous craters/spots with sizes ranging from nano-scales to several microns. The $Pt_{arc\text{-}dep}Ti$ alleviates the CO poisoning effect of methanol electro-oxidation with a higher ratio of the forward anodic peak current (I_f) to the reverse anodic peak current (I_b). The improvement in the catalytic performance should be attributed to that the surrounding Ti sites ameliorate the tolerance to CO adsorption on Pt islands. The $Pt_{arc\text{-}dep}Ti$ electrode reveals its superior electrocatalytic performance toward methanol oxidation and will find promising applications in fields of catalysis, fuel cells and so forth.

14/02225 A numerical method to estimate temperature intervals for transient convection–diffusion heat transfer problems
Xue, Y. and Yang, H. *International Communications in Heat and Mass Transfer*, 2013, 47, 56–61.
This paper presents a numerical method to estimate intervals of temperature for transient convection–diffusion heat transfer problems when uncertainty of thermal parameters is characterized by the interval. A deterministic relationship of interval variables between temperature and thermal parameters is set-up by a Taylor series expansion and the interval analysis, and the lower and upper bounds of temperature can be estimated by a temporally piecewise adaptive algorithm and finite element modelling. A prescribed computing accuracy at each discretized time interval can be achieved via an adaptive process for different size of time step, thus the computing accuracy over the whole time domain can be maintained. A two-dimensional numerical example is provided to verify the proposed approach, and a good accordance can be observed in the comparison of results given by the combinatorial, probability and proposed approaches. The impact of the order of Taylor expansion and the size of time step on the result is discussed.

14/02226 Adaptive soft sensor for online prediction and process monitoring based on a mixture of Gaussian process models
Grbić, R. *et al. Computers & Chemical Engineering*, 2013, 58, 84–97.
Linear models can be inappropriate when dealing with non-linear and multimode processes, leading to a soft sensor with poor performance. Due to time-varying process behaviour it is necessary to derive and implement some kind of adaptation mechanism in order to keep the soft sensor performance at a desired level. Therefore, an adaptation mechanism for a soft sensor based on a mixture of Gaussian process regression models is proposed in this paper. A procedure for input variable selection based on mutual information is also presented. This procedure selects the most important input variables for output variable prediction, thus simplifying model development and adaptation. Apart from online prediction of the difficult-to-measure variable, this soft sensor can be used for adaptive process monitoring. The efficiency of the proposed method is benchmarked with the commonly applied recursive partial least squares and recursive principal component analysis method on the Tennessee Eastman process and two real industrial examples.

14/02227 Agar chemical hydrogel electrode binder for fuel-electrolyte-fed fuel cells
An, L. *et al. Applied Energy*, 2013, 109, 67–71.
This work reports on the synthesis and application of a novel, cost-effective and environmentally friendly agar chemical hydrogel (ACH) electrode binder in fuel-electrolyte-fed fuel cells. The ACH is synthesized by a chemical cross-linking reaction between agar and glutaraldehyde with acetic acid as a catalyst. The fuel cell performance characterization demonstrates that the use of the ACH-based electrode in a fuel-electrolyte-fed fuel cell enables an improvement in cell performance as opposed to the use of conventional Nafion ionomer-based electrodes. The improved performance can be mainly attributed to the enhanced mass/charge transport rendered by the hydrophilic nature and water retention characteristic of agar. This work suggests that the cost-effective ACH binder can replace conventional Nafion ionomers for fuel-electrolyte-fed fuel cells.

14/02228 Analysis of supersonic separators geometry using generalized radial basis function (GRBF) artificial neural networks
Vaziri, B. M. and Shahsavand, A. *Journal of Natural Gas Science and Engineering*, 2013, 13, 30–41.
Supersonic separators (3S) are comprised from unique combination of known physical processes, combining aerodynamics, thermodynamics and fluid dynamics to produce an innovative gas-conditioning process. Condensation and separation at supersonic velocity is the key to achieve a significant reduction in both capital and operating costs. Natural gas dehydration, ethane extraction, liquefied petroleum gas production and natural gas sweetening are some potential applications of 3S units among many others. Feed-forward artificial neural networks (ANNs) are also powerful tools for empirical modelling of various engineering processes. Generalized radial basis function (GRBF) networks which are kernel-based ANNs, have the best approximation property since they represent the optimal solution of multivariate linear regularization theory. A large set of synthetic data are generated in this work via the fundamental modelling of 3S units and are used to train an optimal GRBF network. The trained network is then used to properly design two pilot- and industrial-scale 3S units for natural gas dehumidification processes. Furthermore, the trained network is successfully and much more rapidly used for trend analysis purposes to investigate the effect of various input parameters. The conducted research clearly demonstrates the acceptable performance of such neural networks for both design and trend analysis purposes.

14/02229 Analyzing microcogeneration systems based on LT-PEMFC and HT-PEMFC by energy balances
Jannelli, E. *et al. Applied Energy*, 2013, 108, 82–91.
This paper focuses on the performance analysis of microcogeneration systems based on the integration between a reforming unit (RFU), consisting of a natural gas steam reforming, and a power unit, based on the proton exchange membrane (PEM) fuel cell technology. The analysis has been carried out considering, as power unit, three different PEM fuel cells: a low temperature PEM fuel cell with Nafion™ membrane (LT-FC) operating at 67 °C, a high temperature PEM fuel cell with a membrane based on polybenzimidazole material doped with phosphoric acid (HT-FC1) operating at 160 °C, and a high temperature PEM fuel cell that uses aromatic polyether polymers/copolymers

bearing pyridine units doped with phosphoric acid as electrolyte (HT-FC2) operating at 180 °C. The study has been conducted by using numerical models tuned by experimental data measured in test benches developed at University of Cassino. For sizing the power units able to provide a maximum electric power of 2.5 kW (this size allows to satisfy the electric and thermal energy demand of an Italian household), two designing criteria have been considered. Results have shown that the integrated systems based on the HT-FCs are characterized by high electric efficiency (40%) and cogeneration efficiency (79%). Moreover, the thermal power recovered decreases with the stacks operating temperature, thus the highest cogeneration efficiency (80%) is obtained by the microcogeneration system based on low temperature fuel cells. However, the availability of high temperature heat makes the HT-FC an attractive solution for the cogeneration/trigeneration systems' development.

14/02230 Dielectric and electrical conductivity properties of multi-stage spark plasma sintered HA–$CaTiO_3$ composites and comparison with conventionally sintered materials

Dubey, A. K. *et al. Journal of the European Ceramic Society*, 2013, 33, (15–16), 3445–3453.

One of the different issues limiting the wider application of monolithic hydroxyapatite (HA) as an ideal bone replacement material is the lack of reasonably good electrical transport properties. The comprehensive electrical property characterization to evaluate the efficacy of processing parameters in achieving the desired combination of electroactive properties is considered as an important aspect in the development of HA-based bioactive material. In this perspective, the present work reports the temperature (RT-200 °C) and frequency (100 Hz–1 MHz) dependent dielectric properties and AC conductivity for a range of HA–$CaTiO_3$ (HA–CT) composites, densified using both conventional pressureless sintering in air as well as spark plasma sintering in vacuum. Importantly, the AC conductivity of spark plasma sintered ceramics [$\sim 10^{-5}\,(\Omega\,\mathrm{cm})^{-1}$] are found to be considerably higher than the corresponding pressureless sintered ceramics [$\sim 10^{-8}\,(\Omega\,\mathrm{cm})^{-1}$]. Overall, the results indicate the processing route-dependent functional properties of HA–$CaTiO_3$ composites as well as related advantages of spark plasma sintering route.

14/02231 Effect of bidirectional mass transfer on non-isothermal gas absorption process

Kim, D. S. *International Journal of Thermal Sciences*, 2013, 67, 167–176.

The simultaneous heat and mass process in a binary gas–liquid mixture is modelled by reformulating the classical two-film theory. The original expression from the two-film model is reformulated to obtain algebraic equations where all interfacial quantities are explicitly described in terms of bulk conditions. Use of the new formulation is demonstrated in the analysis of some absorbers operating under various conditions. Influence of various operating parameters is discussed including gas and liquid compositions, liquid pre-cooling, transfer coefficients and flow rates. The new formulation would provide a convenient tool in the analysis of gas–liquid contact devices in general.

14/02232 Enthalpy and temperature of the phase change solid–liquid – an analysis of data of compounds employing entropy

Mehling, H. *Solar Energy*, 2013, 95, 290–299.

Latent heat storage with materials undergoing a phase change solid–liquid is gaining increasing interest due to its potential for applications in energy systems. The demand for optimized storage materials has led to an intensification of materials research in recent years. The research focuses mainly on developing materials with high storage density, and related to this the question what the theoretical limit is. For both it is necessary to understand what affects the melting enthalpy and melting temperature on the atomic and molecular level. In this paper, 1120 different materials (elements and simple chemical compounds) have been analysed to find out what affects the melting enthalpy, entropy, and temperature on the atomic and molecular level. The analysis has been performed plotting data of h_m per atom as a function of s_m/R per atom. While loosening the inter-particle bonds is a necessity for the change of phase from solid to liquid, several other effects have been identified. The most important ones are a change of bond type between the solid and the liquid phase, and a change of the particle structure, which is equal to a chemical reaction. The latter shows that latent heat storage employing a phase change solid–liquid can include a chemical reaction.

14/02233 Experimental analysis of combustion assisted gravity drainage

Rahnema, H. *et al. Journal of Petroleum Science and Engineering*, 2013, 103, 85–96.

Combustion-assisted gravity drainage (CAGD) is a new enhance oil recovery process that uses dual horizontal wells for the injection of air and the production of heavy oil. One of the important features of CAGD is the properly oriented dual horizontal wells, similar to steam-assisted gravity drainage (SAGD), which assists in the development of combustion chamber and stable growth of the combustion front in the reservoir. This research evaluates the potential of CAGD as an attractive alternative to conventional *in situ* combustion (ISC). A three-dimensional laboratory model was designed and constructed to study the CAGD process. The combustion cell was fitted with 48 thermocouples. A horizontal producer was placed near the base of the model with a horizontal injector in the upper part. The CAGD process combines the advantages of both gravity drainage and the conventional ISC. Experimental results showed the combustion chamber developed in the wide area of the porous media around the horizontal injector. This combustion chamber consisted of flue gases, injected air and hot oil. The gravity drainage is the main mechanism for oil production and extracting the flue gases from reservoir. Recorded temperatures reached up to 650 °C at the combustion front, with oil recovery more than 82% original oil in place. Experimental data showed that improper well distance could cause severe plugging in production well perforations and terminate the process prematurely.

14/02234 Functional sensitivity of testing the environmental Kuznets curve hypothesis

Wang, Y.-C. *Resource and Energy Economics*, 2013, 35, (4), 451–466.

Conventional tests for the environmental Kuznets curve (EKC) hypothesis mostly apply a quadratic equation in modelling the non-linear relationship between environmental indices (such as air pollutants) and welfare measures (such as income per capita). If their inverted-U shaped pattern is empirically accepted with two significant regressors, the income per capita and its square transformation, the EKC hypothesis is supported. Using an Organization of Economic Cooperation and Development (OECD) sample, this paper shows that the validity of testing the EKC hypothesis is sensitive to how income is transformed non-linearly in sulfur and carbon EKC regressions. This paper carries out experiments on different powers of γ for transforming income non-linearly and concludes that only when $0 < \gamma < 1$ and $1 < \gamma < 2$ will the EKC regression demonstrate a testable non-linear cointegration relationship between the two air pollutants and income per capita. In the generalized EKC regressions estimated in this paper, although sulfur and carbon EKC patterns were found in the OECD sample, none of the EKC regressions using different γ is a cointegrating equation. This finding implies an inside critique to the EKC literature that failure of cointegration of the conventional EKC regression is not because of using the quadratic functional form, but because of the fundamentally spurious relationship between the trends of pollutants and income levels.

14/02235 Generation of operating procedures for a mixing tank with a micro genetic algorithm

Batres, R. *Computers & Chemical Engineering*, 2013, 57, 112–121.

This paper explores the use of a micro genetic algorithm that uses variable-length chromosomes and a seeding scheme based on tabu search. The problem is to find the sequence of actions that have to be executed in the shortest time possible, but also in a way that minimizes the possibility of situations that may endanger the plant personnel and plant facilities. The proposed approach was tested on the generation of the optimum sequences for start-up and shutdown of a mixing vessel similar to the equipment used in the synthesis of acrylic acid. The results show that the proposed method outperforms the traditional genetic algorithm both in terms of the quality of the solution and computational effort.

14/02236 Hydrodynamics of gas–liquid micro-fixed beds – measurement approaches and technical challenges

Faridkhou, A. *et al. Chemical Engineering Journal*, 2013, 223, 425–435.

Despite many areas that are open to investigation in the hydrodynamic study of micro-fixed bed reactors, conducting research in this field is mostly hampered by a number of experimental challenges that have made many attempts ineffectual. This work provides a summary of the technical challenges, problems and misconstrues one might encounter in performing hydrodynamic experiments on micro-fixed bed reactors. Some of these issues will be pointed out upon comparing classical residence time distribution (RTD) measurements through electrical conductivity probes at micro-fixed bed scale with near-wall RTD obtained via visualizations of dye-tracer elution and monitoring the changes in grey level intensity of the images. Laterally-averaged grey level intensity at both upstream and downstream extremities of the wall regions of interest acted as inlet and outlet curves for the Aris method. The major outcome of this work was experimental confirmation of theoretically predicted maximum liquid velocity in the high porosity zone close to the wall. Finally, the experimental results on pressure drop and liquid holdup obtained on following the right experimental protocols are presented.

14/02237 Impact of liquid driving flow on the performance of a gas-inducing impeller

Wang, Z. *et al. Chemical Engineering and Processing: Process Intensification*, 2013, 69, 63–69.

This study was conducted to improve the gas-induction performance over a preliminary gas-inducing impeller designed in a previous work. For the first time, a series of liquid-inlet holes with different diameters were drilled separately so as to examine their effects on the gas-induction process and also to find the optimum size. The critical impeller speed (N_{CG}) and the overall gas hold-up (ε_G) were measured experimentally in order to evaluate the properties of the gas-inducing impeller. A mathematical model, which takes into account the geometrical parameters of the gas-inducing impeller, was proposed to predict N_{CG} of the gas-inducing impeller with or without liquid-inlet holes. The predictions are in good agreement with the experimental results. The results also show that the optimum gas-induction properties would be obtained with respect to the lowest value of N_{CG} and the highest value of ε_G, when the diameter of the liquid-inlet hole is approximately 0.5 times the diameter of the gas-inducing pipe.

14/02238 Intercomparative tests on phase change materials characterisation with differential scanning calorimeter

Lazaro, A. *et al. Applied Energy*, 2013, 109, 415–420.

For the correct design of thermal storage systems using phase change materials (PCMs) in any application, as well as for their simulation, it is essential to characterize the materials from thermophysical and rheological standpoints (phase change enthalpy, thermal conductivity in solid and liquid phases, viscosity and density in function of temperature). Taking advantage of the different research groups facilities available in two international networks: within the International Energy Agency, the Energy Conservation through Energy Storage IA implementing agreement and Solar Heating and Cooling programme Task 42/Annex 24 'Compact thermal energy storage – material development for system integration', and the COST Action TU0802 'Next generation cost effective phase change materials for increased energy efficiency in renewable energy systems in buildings (NeCoE-PCM)' a set of round-robin tests was proposed. The objective was to come to comparable results for PCMs using differential scanning calorimetry to determine their melting enthalpy as well as their melting and solidification behaviour. The first round-robin test was without defining the procedure, the second one with a predefined procedure for the measurements, but not for calibration and the third one with a predefined procedure for calibration, for the measurements and also for the data evaluation. The main conclusion of the paper is that enthalpy in function of temperature determined using a dynamic method for DSC can be influenced by certain reasons and finally a methodology to avoid these influences have been proposed.

14/02239 Longitudinal wave propagation in multiwalled carbon nanotubes

Aydogdu, M. *Composite Structures*, 2013, 107, 578–584.

The longitudinal wave propagation in multiwalled carbon nanotubes is investigated using the non-local elasticity theory. A multiwalled rod model is proposed in the formulation. The van der Waals force is considered in the axial direction. The effect of various parameters like the radius of nanotubes, van der Waals forces and non-local parameters on the longitudinal wave propagation in multiwalled carbon nanotubes is discussed. It is obtained that different axial relative motion may exist in double-walled carbon nanotubes. The present results can be useful in the design of nanoscale linear motors, oscillators and similar nanoscale electromechanical systems.

14/02240 Modular object-oriented methodology for the resolution of molten salt storage tanks for CSP plants

Rodríguez, I. *et al. Applied Energy*, 2013, 109, 402–414.

Two-tank molten salt storages are the most widespread thermal energy storage technology within concentrated solar power (CSP) plants. In spite of this, there are design aspects such as thermal losses control, optimization of the storage or how these devices scale up with the increase in power capacity of the plant which still should be considered. In this sense, numerical modelling of these systems can be a powerful tool for reducing their cost. The present work aims at modelling molten salt tanks by proposing a parallel modular object-oriented methodology which considers the different elements of the storage (e.g. tank walls, insulation material, tank foundation, molten salt storage media, etc.) as independent systems. Each of these elements can be solved independently and using different levels of modelling (from global to fully three-dimensional models), while at the same time they are linked to each other through their boundary conditions. The mathematical models used, together with some illustrative examples of the application of the proposed methodology, are presented and discussed in detail.

14/02241 Novel packaging design for high-power GaN-on-Si high electron mobility transistors (HEMTs)

Cheng, S. and Chou, P.-C. *International Journal of Thermal Sciences*, 2013, 66, 63–70.

This study describes the development of packaging for high-power AlGaN/GaN high electron mobility transistors (HEMTs) on a silicon substrate. A transistor is attached to a V-grooved copper base, and mounted on a TO-3P lead-frame. Unlike flipchip or copper–molybdenum–copper (CMC)-based packaging technology, which is popular in the GaN HEMT industry, the proposed packaging structure is implemented on the periphery of the surface of the device to promote thermal dissipation from the Si substrate. The various thermal paths from the GaN gate junction to the case dissipate heat by spreading it to a protective coating; transferring it through bond wires; spreading it laterally throughout the device structure through an adhesive layer, and spreading it vertically through the bottom of the silicon chip. The effects of the design of the structure and its fabrication process on the performance of the device and its thermal resistance were studied. Thermal characterization reveals that the thermal resistance from the GaN chip to the TO-3P package was 13.72 °C/W. Self-heating in AlGaN/GaN device structures was measured by infrared thermography and micro-Raman spectroscopy. Experimental results indicated that a single chip that was packaged in a 5×3 mm V-grooved Cu base with a total gate-periphery of 30 mm had a power dissipation of 22 W with a drain bias of 100 V. Both DC and pulsed current–voltage (I_D–V_{DS}) characteristics are measured for a range of transistor structures and sizes, at various of power densities, pulse lengths, and duty factors. These are compared with measured channel temperature profiles.

14/02242 Quaternary plutonic magma activities in the southern Hachimantai geothermal area (Japan) inferred from zircon LA-ICP-MS U–Th–Pb dating method

Ito, H. *et al. Journal of Volcanology and Geothermal Research*, 2013, 265, 1–8.

In order to constrain the timing of plutonic magma emplacements relevant to current geothermal activity in the Hachimantai geothermal area, north-east Japan, laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) U–Th–Pb analyses were performed on zircons from two different origins. One is from the quaternary Kakkonda granite in the Kakkonda geothermal field, whose present temperature at ~3700 m depth is 500 °C, and the other is from a clastic dike in the Matsukawa geothermal field. Zircons from the Kakkonda granite were obtained at a depth of 1998 m and their ^{238}U–^{206}Pb and U–Th ages showed ~0.1 Ma, which probably indicates that the Kakkonda granite is the world's youngest emplaced granitic magma body ever confirmed. The clastic dike in the Matsukawa geothermal field contains dioritic to tonalitic xenoliths; therefore zircons extracted from the dike should also be of plutonic origin. ^{238}U–^{206}Pb age of 1.08 ± 0.08 Ma (after correction for initial ^{230}Th disequilibrium; error shown as 95% confidence level) was obtained from the zircons. Therefore it was found that there were at least two Quaternary plutonic magma activities (~1.1 and ~0.1 Ma) in the Hachimantai geothermal area. Through this study, it was also found that U–Th–Pb dating using a quadrupole type ICP-MS coupled with excimer laser is applicable to Quaternary zircons as young as 0.1 Ma and Fish Canyon Tuff zircon is usable as a standard material for U–Th–Pb dating method.

14/02243 Regime mapping and the role of the intermediate region in wall-coated microreactors

Lopes, J. P. *et al. Chemical Engineering Science*, 2013, 94, 166–184.

Operation of a wall-coated microreactor can occur in several mass transfer-reaction regimes. This study defines these regimes analytically in several planes of a multi-parametric map, taking into account the different degrees of concentration profile development, as well as the influence of non-unity orders of reaction and reactant inhibition in the kinetic law. It was found that the regions where conversion can be calculated from simplified mass transfer models are not discriminated by common results for entrance-length. The authors also illustrate the trade-offs that exist across this operating map concerning the catalyst design (costs associated with loading and volume) and overall system performance (evaluated in terms of reactant conversion, flow efficiency and microreactor effectiveness). It is shown that under certain conditions, the existence of moderate mass transfer resistance can be advantageous (even if internal limitations cannot be avoided), clarifying the role of the intermediate transport-reaction region.

14/02244 Sorption isotherms of mixtures of polymers, proteins and electrolytes – measurement data and model predictions

Kachel, S. *et al. Chemical Engineering and Processing: Process Intensification*, 2013, 68, 45–54.

Blends of water-soluble polymers and proteins serve as a matrix for the immobilization of active components in coatings. Water absorption of these blends is important for the properties and the performance of the films. The authors propose an additive model for the calculation of

water absorption into polymer blends that is able to describe the measured values for different concentrations and for different classes of additives. Sorption isotherms of the polymers polyvinylalcohol and polyvinylpyrrolidone, the protein bovine serum albumin and the salt sodium chloride were gathered using an automated gravimetric sample exchanger. The resulting sorption isotherms were modelled using the Flory–Huggins model for polymers and protein and an activity coefficient model for the salt. Sorption isotherms of mixtures were calculated using a model of weighted sums for the absorbed water. The prediction was able to describe the measured values with a deviation factor close to 1 above a water mass fraction of 0.1 in the film. For lower water mass fractions the relative deviations were larger due to the small values for the water absorption. This predictive model reduces the number of experiments necessary for the determination of sorption isotherms of mixtures.

14/02245 Stirred tank membrane emulsification using flat metallic membranes: a dimensional analysis

Suárez, M. A. *et al. Chemical Engineering and Processing: Process Intensification*, 2013, 69, 31–43.

The performance of a membrane emulsification unit, using flat membranes in a stirred tank, has been examined by dimensional analysis. The dimensionless numbers were defined in terms of shear and membrane pore size. Dimensionless droplet size prediction models based on simple force balances were used to select the most representative dimensionless numbers including operating parameters. Oil-in-water emulsions were produced with tailor-made metallic membranes with pore sizes of 30 and 50 μm. Results showed that monodisperse emulsions were produced with span values around 0.5, significantly lower than when a rotor-stator homogenizer is used. The influence of the selected operating parameters (impeller rotational speed, continuous phase viscosity and dispersed phase flux) on droplet size distribution was studied and experimental results were compared with droplet size prediction models. Impeller rotational speed and membrane pore size were the key parameters influencing emulsion droplet size and monodispersity. A correlation based on the Euler dimensionless number, including all the operating parameters is proposed.

14/02246 Stochastic comparison between simplified energy calculation and dynamic simulation

Kim, Y.-J. *et al. Energy and Buildings*, 2013, 64, 332–342.

For building energy performance prediction and assessment, two approaches are widely used: simplified calculation (e.g. ISO 13790) and dynamic simulation (e.g. EnergyPlus). The ISO 13790 standard uses simple algebraic equations, while dynamic simulation is focused on transient behaviour of systems and buildings. This study aims to compare the aforementioned two approaches under uncertainty. For this study, an office building was selected and modelled using ISO 13790 and EnergyPlus 6.0 with the assumptions as close to each other as possible. The sensitivity analysis was employed to identify unknown inputs that have important bearing on the simulation output. Then, Latin hypercube sampling (LHS) method, one of the Monte Carlo techniques, was employed for uncertainty propagation. It was found that the two approaches (ISO 13790 vs EnergyPlus) have different population means from each other and require careful calibration for utilization factors in the simplified approach (reference numerical parameter, reference time constant for both heating and cooling). To calibrate the unknown parameters in the simplified approach, Bayesian calibration was applied in this study. Bayesian calibration is useful to obtain the posterior distribution for the unobserved quantities based on the presumed prior distribution. It is concluded that the simplified approach, when stochastically calibrated, becomes surprisingly similar to the dynamic simulation.

14/02247 Strategies for enhancing electrochemical activity of carbon-based electrodes for all-vanadium redox flow batteries

Flox, C. *et al. Applied Energy*, 2013, 109, 344–351.

Two strategies for improving the electroactivity towards VO^{2+}/VO_2^+ redox pair, the limiting process in all-vanadium redox flow batteries (VFBs), were presented. $CuPt_3$ nanoparticles supported onto graphene substrate and nitrogen and oxygen polyacrylonitrile (PAN)-functionalized electrodes materials have been evaluated. The morphology, composition, electrochemical properties of all electrodes prepared was characterized with field emission-scanning electrode microscopy, X-ray photoelectron spectroscopy, cyclic voltammetry, electrochemical impedance spectroscopy and cell charge–discharge test. The presence of the $CuPt_3$ nanocubes and nitrogen and oxygen functionalities enhance the electrocatalytic activity of the electrodes materials accelerating the oxygen and electron transfer processes. The battery performance was also evaluated using PAN-functionalized electrodes exhibiting a high of energy efficiency of 84% (at current density 20 mA cm^{-2}) up to thirtieth cycle, indicating a promising alternative for improving the VFB.

14/02248 The generalized embedded atom model of interatomic interaction and its application to α-Pu

Ionov, G. V. *et al. Journal of Nuclear Materials*, 2013, 435, (1–3), 10–16.

The generalized embedded-atom model (GEAM) for interatomic interaction in metals with complex electronic and crystal structure has been developed as a modification of the angular dependence term of well-known MEAM potential. Here, the authors present an analytical form of the new interatomic potential, including partial forces ready to be implemented into MD computer code. The new model has been applied to low-temperature monoclinic α-phase of plutonium. In rather long MD simulations with flexible unit cell geometry it has been shown that monoclinic lattice proved to be mechanically stable in temperature range 0–300 K and at zero stress tensor. Results of MD simulations obtained with the new model at finite temperatures were compared with experimental and *ab initio* data on the properties of the material.

14/02249 Thermodynamic efficiency of synthesis, storage and breakdown of the high-energy metabolites by photosynthetic microalgae

Sorgüven, E. and Özilgen, M. *Energy*, 2013, 58, 679–687.

Lipids and carbohydrates are employed in nature to store energy through their large number of high-energy atomic bonds in their structure. The internal energy stored in these bonds is used to fuel work-producing engines or metabolic activity of living organisms. This paper investigates the thermodynamic efficiency of the glucose and lipid synthesis and breakdown by photosynthetic microalgae. Photosynthetic microalgae are able to convert 3.8% of the solar exergy into the chemical exergy of algal lipid. As the microalgae convert the first product of the photosynthesis, i.e. glucose, into lipids, 47–49% of the chemical exergy is lost. If the microalgal cell consumes the photosynthetically produced glucose for its own energy demand, then about 30% of the glucose exergy can be converted into work potential in case of immediate and short-term energy demands. Organisms can convert about 22% of the glucose exergy into work potential after long-term storage. If the algal lipid is harvested for biodiesel production and the produced biodiesel is combusted in a diesel engine, then about 17% of the exergy of the photosynthetically produced glucose can be converted into useful work. Biodiesel is among the most popular renewable fuels. The lipids are harvested from their storage in the cells to produce biodiesel before following the lipid breakdown path of the cellular metabolism. This analysis indicates that, extracting the first product of photosynthesis, i.e. glucose or glucose polymers instead of lipids may be more efficient thermodynamically, if new motors that are capable of extracting their bond energy are developed.

Fuel cell technology

14/02250 Anodic current distribution in a liter-scale microbial fuel cell with electrode arrays

Zhang, L. *et al. Chemical Engineering Journal*, 2013, 223, 623–631.

A litre-scale microbial fuel cell with graphite rod electrode arrays (MFC-EA) was constructed and its relative anodic current distribution was investigated with nine groups of anode electrodes. Meanwhile, the influences of chemical oxygen demand (COD) concentration and ionic strength of anolyte on anodic current distribution were discussed. It is demonstrated that the electrode spacing between the anode segment and cathode significantly influenced the ohmic resistance distribution and the biomass content of each segment, further affected the anodic current distribution. A significantly uneven current distribution was found in MFC-EA, especially at high currents. The further the anode segment was away from the cathode, the smaller the segment current generation contributed to the total current. Consequently, a suitable MFC structure with equidistant electrode spacing will be a necessary consideration for large-scale MFC design. Moreover, for MFC-EA, improvement on the uneven current distribution was achieved by feeding the anolyte with a COD concentration of 1000 mg COD L^{-1} or with 0.2 M KCl.

14/02251 Assessment of bioelectricity production in microbial fuel cells through series and parallel connections

Jafary, T. *et al. Energy Conversion and Management*, 2013, 75, 256–262.

Microbial fuel cell (MFC) units that are connected in series and parallel, may increase MFC performance in forms of voltage and current respectively. In this research, three individual MFC units were connected with different concentrations (10, 20 and 30 g l^{-1}) of glucose, fructose and sucrose. Generated power and current were analysed through polarization and voltage curves. Parallel connections of three units, which fed with 10 g l^{-1} of each substrate, resulted in voltage and power densities of 0.65 V and 72.77 mW m^{-2}, respectively. This

configuration produced a current density of 191.36 mA m^{-2} which was approximately three times higher than a single unit. By using a similar configuration but in series, the voltage produced was increased to 1.78 V, as long as power and current densities were about at the same level of one single unit (52.35 mW $m^{-2}$and 57.6 mA m^{-2}). Substrate concentration enhancement to 20 and 30 g l^{-1} resulted in the same magnitude of increase for cell performances compared to the single unit results. Serial connection of 20 g l^{-1} of three substrates (glucose, fructose and sucrose) showed the highest results compared to other understudied substrate concentrations; 109.45 mW m^{-2} of power density, 98.14 mA m^{-2} of current density and 2.042 V as voltage. Shift of MFC configuration to parallel connection demonstrated 381.44 mA m^{-2}, 128.72 mW m^{-2} and 0.68 V as current, power densities and voltage respectively. This configuration corresponds to the lowest calculated internal resistance.

14/02252 Decentralized combined heat and power production by two-stage biomass gasification and solid oxide fuel cells

Bang-Møller, C. *et al. Energy*, 2013, 58, 527–537.

To investigate options for increasing the electrical efficiency of decentralized combined heat and power (CHP) plants fuelled with biomass compared to conventional technology, this research explored the performance of an alternative plant design based on thermal biomass gasification and solid oxide fuel cells (SOFC). Based on experimental data from a demonstrated 0.6 MW_{th} two-stage gasifier, a model of the gasifier plant was developed and calibrated. Similarly, an SOFC model was developed using published experimental data. Simulation of a 3 MW_{th} plant combining two-stage biomass gasification and SOFCs predicted a net electrical efficiency of 44.9% (lower heating value) when 1.4 MWe power was produced. The work had significant focus on providing a highly accurate model of the complete plant. A sensitivity analysis revealed that the SOFC operating temperature, SOFC fuel utilization factor, carbon conversion factor in the gasifier and the efficiency of the DC/AC inverter were the most influential parameters in the model. Thus, a detailed study of the practical values of these parameters was conducted to determine the performance of the plant with the lowest possible uncertainty. The SOFC fuel utilization will in practice be based on a balance between efficiency and lifetime of the SOFC and is thus a decision of the plant design.

14/02253 Development of a continuous hydrogen generator fueled by ammonia borane for portable fuel cell applications

Kim, Y. *et al. Journal of Power Sources*, 2013, 229, 170–178.

Thermally induced dehydrogenation from a mixture of ammonia borane (AB) and a chemical promoter, tetraethyleneglycol dimethylether (T4EGDE) (AB:T4EGDE = 79 : 21, wt%) has been demonstrated as an efficient method for hydrogen production at 85–145 °C. The authors build on these prior results to create a continuous H_2 generator fuelled by solid AB beads. The as-developed H_2 generator releases *ca.* 2 equiv of hydrogen autothermally during operation by utilizing excess heat produced from AB dehydrogenation without any external heater. A purifying system equipped with acidic filter materials is further utilized to remove gaseous byproducts other than hydrogen. The H_2 generator shows a rapid H_2-release rate up to 3.3 l(H_2) min^{-1} with fast load-following capability. The as-developed H_2 generator is ultimately integrated with a commercial 200 W_e polymer electrolyte membrane fuel cell (PEMFC) to test its capability.

14/02254 Effects of surface microstructures of gas diffusion layer on water droplet dynamic behaviors in a micro gas channel of proton exchange membrane fuel cells

Chen, L. *et al. International Journal of Heat and Mass Transfer*, 2013, 60, 252–262.

Numerical simulations using volume of fluid (VOF) method are performed to investigate the effects of the surface microstructures of gas diffusion layer (GDL) on the dynamic behaviours of a water droplet in a micro-gas channel (GC) of proton exchange membrane fuel cells (PEMFCs). The detachment size of a droplet under different air velocity and GDL wettability is investigated. Simulation results show that the microstructures of the GDL surface indeed affect the dynamics of water droplets. The directional distributions of carbon fibres in the flow direction are desirable for detaching droplets from the GDL surface and reducing flooding in GC. In addition, a force analytical model is developed, which takes into account the effects of microstructures of GDL surface as well as the surface tension force due to droplet deformation with some simplified assumptions. It is found that surface tension force due to the droplet deformation cannot be simply ignored when analysing forces acting on the droplet, as the contact angle hysteresis is usually relatively large.

14/02255 Electrochemical–thermal analysis of 18650 lithium iron phosphate cell

Saw, L. H. *et al. Energy Conversion and Management*, 2013, 75, 162–174.

In this study, a pseudo two-dimensional electrochemical model was coupled with a lumped thermal model to analyse the electrochemical and thermal behaviour of the commercial 18650 lithium iron phosphate battery. The cell was cut to obtain the physical dimension of the current collector, electrodes, separator, casing thickness, gasket, etc. The layer structure of the spiral wound, cylindrical casing, gasket and heat shrink-wrapping were modelled to understand better the temperature distribution across the cell. Natural convection and radiation were used to reflect the heat dissipation on the side surface. Experimental study was carried out to validate the simulation results. The simulation results suggested that the cell temperature and total heat generation rate have a positive correlation with the I_t-rates and these were in line with the experimental results. Reaction heat was the main heat source and it contributed about 80–85% of the total heat generated during charging and discharging of the cell. Based on the simulation results, the final temperature of the cell surface was elevated to 59 °C using $10I_t$ of charging. The effect of electrical contact resistance between the connectors and terminals of the cell was also investigated. It was found that the electrical contact resistance caused a large temperature gradient across the cell. These effects are important and should be considered in the design of an electric vehicle's battery pack and thermal management system to reduce the maximum temperature and maintain the temperature uniformity of the cells.

14/02256 Non-isothermal modeling of a small passive direct methanol fuel cell in vertical operation with anode natural convection effect

Wang, L. *et al. Energy*, 2013, 58, 283–295.

A two-dimensional, non-isothermal model is presented for a small passive direct methanol fuel cell (DMFC) in vertical operation. The effect of natural convection at the anode in the fuel reservoir is considered. The coupled heat and mass transport of the whole cell, along with the electrochemical reactions occurring in the passive DMFC are modelled. The comprehensive model is solved numerically by the finite element method and validated against the experiment results reported in this paper. The numerical results show that when in vertical operation, the cell temperature increases gradually from the bottom of the cell to the top of the cell, resulting from natural convection at the anode. A higher cell temperature will lead to stronger natural convection in the fuel reservoir, which will in turn lead to a larger temperature difference across the cell. The results also indicate that the rate of methanol crossover increases with increasing methanol concentration from 1 to 4 M. When incrementally increasing the current densities, the rate of methanol crossover decreased at low methanol concentration of 1–2 M but increased at high methanol concentration of 3–4 M.

14/02257 One-dimensional manganese oxide nanostructures as radical scavenger to improve membrane electrolyte assembly durability of proton exchange membrane fuel cells

Lei, M. *et al. Journal of Power Sources*, 2013, 230, 96–100.

One-dimensional manganese oxide (MnO_2) scavengers are proposed to minimize the radical degradation of membrane electrode assembly (MEA) in fuel cells. The synthesized MnO_2 nanotubes and MnO_2 nanowires are *ca.* 5–8 nm in diameter and more than 100 nm in length, respectively. Water retention of the hydrophilic MnO_2 reduces the humidity sensitivity of the fuel cells. At 75 RH% humidify levels of inlet gas at 60 °C, single cells assembled by catalyst layer with MnO_2 nanotubes and nanowires as the cathodes have peak power densities of 599.3 and 536.8 mW cm^{-2}, respectively. Radical scavenger MnO_2 in the cathode catalyst is effective in minimizing the radical degradation in proton exchange membrane (PEM) fuel cells. After the OCV degradation, the hydrogen crossover of cell assembled by catalyst layer with MnO_2 nanowires or MnO_2 nanotubes in anode and traditional catalyst layer in cathode are about 5.3 and 4.9 mA cm^{-2}, respectively. As a comparison, single cell with conventional catalyst layer in both anode and cathode, the hydrogen crossover through the MEA is increased to 14.7 mA cm^{-2}.

14/02258 Prediction of the theoretical capacity of non-aqueous lithium-air batteries

Tan, P. *et al. Applied Energy*, 2013, 109, 275–282.

In an attempt to realistically assess the high-capacity feature of emerging lithium-air batteries, a model is developed for predicting the theoretical capacity of non-aqueous lithium-air batteries. Unlike previous models that were formulated by assuming that the active materials and electrolyte are perfectly balanced according to the electrochemical reaction, the present model takes account of the fraction of the reaction products (Li_2O_2 and Li_2O), the utilization of the onboard lithium metal, the utilization of the void volume of the

porous cathode, and the onboard excess electrolyte. Results show that the gravimetric capacity increases from 1033 to 1334 mA h/g when the reaction product varies from pure Li_2O_2 to pure Li_2O. It is further demonstrated that the capacity declines drastically from 1080 to 307 mA h/g when the case of full utilization of the onboard lithium is altered to that only 10% of the metal is utilized. Similarly, the capacity declines from 1080 to 144 mA h/g when the case of full occupation of the cathode void volume by the reaction products is varied to that only 10% of the void volume is occupied. In general, the theoretical gravimetric capacity of typical non-aqueous lithium-air batteries falls in the range of 380–450 mA h/g, which is about 10–12% of the gravimetric capacity calculated based on the energy density of the lithium metal. The present model also facilitates the study of the effects of different parameters on the mass and volume change of non-aqueous lithium-air batteries.

14/02259 Thermal control and performance assessment of a proton exchanger membrane fuel cell generator
Hwang, J.-J. *Applied Energy*, 2013, 108, 184–193.
An original-designed thermal control scheme that manages the thermal behaviours in a proton exchange membrane (PEM) fuel cell generator has been proposed. It not only keeps the stack from overheating under extreme high external loads, but also prevents the stack from staying too cold in the cold-start conditions. A thermal control unit (TCU) together with a smart control algorithm is able to limit the fuel cell operation temperature in a desired range. The TCU comprises mainly a thermostat, a radiator, and a heater. It divides the stack coolant into a cooling stream and a heating stream that maintains a pre-set coolant temperature before entering the stack. Parametric studies include the external loads ($0 < P_L < 4$ kW) and the stack coolant inlet temperature (SCIT = 53, 58 and 63 °C). The dynamics of SCIT under different loads are measured to verify the thermal reliability of the fuel cell generator. Then, examining the effect of SCIT on the system efficiency assesses the performance the fuel cell generator. Finally, an empirical correlation for the system efficiency of the PEM fuel cell generator under different SCITs is presented as a function of the external loads.

14/02260 Vacuum-assisted drying of polymer electrolyte membrane fuel cell
Tang, H.-Y. *et al. Applied Energy*, 2013, 107, 264–270.
Purging a polymer electrolyte membrane fuel cell (PEMFC) with dry N_2 to remove water in the catalyst layer and the membrane during shutdown is necessary for ensuring successful startup and avoiding damages from the freeze/thaw cycling during cold-start. However, carrying N_2 onboard may be impractical for mobile applications. Vacuum-assisted drying can accelerate and aid in water removal by reducing the boiling point of water, thus enhancing the evaporation and diffusion rate. This method is applied to a single cell PEMFC and compared to purging using dry N_2. The drying process was monitored using electrochemical impedance spectroscopy, and the results were fitted to an equivalent circuit model. These experimental results show the vacuum-assisted drying method may provide faster and more thorough water removal than N_2 purging.

15 ENVIRONMENT

Pollution, health protection, applications

14/02261 A thousand flowers blooming? An examination of community energy in the UK
Seyfang, G. *et al. Energy Policy*, 2013, 61, 977–989.
Community energy has been proposed as a new policy tool to help achieve the transition to a low-carbon energy system, but the evidence base for this strategy is partial and fragmented. The authors therefore present new empirical evidence from the first independent UK-wide survey of community energy projects. This survey investigates the objectives, origins and development of these groups across the UK, their activities and their networking activities as a sector. The authors also examine the strengths and weaknesses of these groups, along with the opportunities and threats presented by wider socioeconomic and political contexts, in order to improve understanding of the sector's potential and the challenges it faces. They highlight several key issues concerning the further development of the sector. First, this highly diverse sector is not reducible to a single entity; its multiple objectives need joined-up thinking among government departments. Second, its civil society basis is fundamental to its success at engaging local communities, and makes the sector quite distinct from the large energy companies these community groups are aiming to work alongside. There are inherent tensions and vulnerabilities in such a model, and limits to how much these groups can achieve on their own: consistent policy support is essential.

14/02262 Building low carbon communities in China: the role of individual's behaviour change and engagement
Jiang, P. *et al. Energy Policy*, 2013, 60, 611–620.
Low carbon sustainability has been addressed in China's national development strategies. This research explores individual behaviour change and engagement in building low carbon communities in China through a case study looking at the building of a low carbon campus at Fudan University, Shanghai. Individual behaviour directly influences the overall energy consumption and carbon emissions on Fudan University's campus. Even though relevant polices have been issued for energy conservation, the energy consumption increased by 5% every year, which suggests that the 'top-down' approach telling students and staff 'what to do' does not work effectively. Based on a comprehensive method which includes the individual and social aspects related to the energy behaviour, the research analyses the promotion of individual engagement in building a low carbon campus through behaviour change based on four main aspects: (1) awareness raising and behaviour forming; (2) approaches to encourage behaviour change; (3) beyond the barriers and the constraints and (4) systems and mechanisms for the long-term engagement. A low carbon management system is proposed for not only addressing management and technical solutions at the university level, but also based on the contributions from behaviour changes in establishing a low carbon campus at Fudan University at the individual level.

14/02263 Efficiency of combined FTIR and Raman spectrometry for online quantification of soil gases: application to the monitoring of carbon dioxide storage sites
Taquet, N. *et al. International Journal of Greenhouse Gas Control*, 2013, 12, 359–371.
This study reports the ability of the coupled Raman–Fourier transform infrared (FTIR)/completion system to establish continuous measurements of soil gases for the monitoring of the CO_2 sequestration sites. The method was deployed in the first French carbon dioxide capture and storage pilot at Lacq-Rousse, in France during the injection operation. In this study, the continuous recording of the N_2, O_2, H_2O and CO_2 concentrations in soil allowed by the coupled Raman/FTIR completion system appears as a first step to decipher CO_2 abnormal variations at the surface of the CCS site.

14/02264 Emission taxes and the adoption of cleaner technologies: the case of environmentally conscious consumers
Gil-Moltó, M. J. and Varvarigos, D. *Resource and Energy Economics*, 2013, 35, (4), 486–504.
This study models a market with environmentally conscious consumers and a duopoly in which firms consider the adoption of a clean technology. The authors show that as pollution increases, consumers shift more resources to the environmental activities, thereby affecting negatively the demand faced by the duopoly. This effect generates incentives for firms to adopt the clean technology even in the absence of emissions taxes. When such taxes are considered, the results indicate that the benefit of adopting the clean technology is initially increasing and then decreasing in the emission tax. The range of values for which the emission tax increases this benefit becomes narrower when the consumers' environmental awareness is stronger.

14/02265 Energyscapes: linking the energy system and ecosystem services in real landscapes
Howard, D. C. *et al. Biomass and Bioenergy*, 2013, 55, 17–26.
The drive for sustainable energy production is leading to increased deployment of land-based renewables. Although there is public support, in principle, for renewable energy at a national level, major resistance to renewable energy technologies often occurs at a local level. Within this context, it can be useful to consider the 'energyscape' which is initially define as the complex spatial and temporal combination of the supply, demand and infrastructure for energy within a landscape. By starting with a consideration of the energyscape, the positive and negative interactions with other ecosystem services within a particular landscape can then be considered. This requires a multi-disciplinary systems-approach that uses existing knowledge of landscapes, energy options, and the different perspectives of stakeholders. The approach is examined in relation to pilot case-study comprising a 155 km^2 catchment in Bedfordshire, England.

14/02266 Environmental impact assessment of a turboprop engine with the aid of exergy
Atilgan, R. *et al. Energy*, 2013, 58, 664–671.

To develop approaches that effectively reduce engine environmental effect of aircraft, it is necessary to understand the mechanisms that have enabled improvements in thermodynamic efficiency of aircraft engines. In this work, a turboprop engine used in regional aircraft that produces 1948 shp and 640 N m torque is examined using exergo-environmental method. The results show compressor, combustion chamber, gas generator turbine, power turbine and exhaust nozzle create 9%, 69%, 13%, 7%, 2% of total environmental impact of the engine, respectively. According to rates, the compressor and gas turbine can be considered first to improve in case of component related environmental impact. Furthermore, total component related environmental impact for the turboprop engine is found to be 2.26 mPts/s for the constructional phase and 2.34 mPts/s for the operation/maintenance phases. Accordingly, it is suggested that, in order to estimate environmental impact metric of aircrafts, the exergo-environmental analysis can be employed for aircraft propulsion systems.

14/02267 Environmental impact of decentralized power generation in Santa Clara City, Cuba: an integrated assessment based on technological and human health risk indicators

Herrera, I. *et al. Applied Energy*, 2013, 109, 24–35.

At present the worldwide energy market is dominated by fossil fuels, despite that it has been demonstrated to be a major source of environmental problems. In Cuba, about 96% of the power generation comes from fossil fuels, and 26% of this is produced by decentralized power stations (DPSs). DPS technology grew by a factor of six from 2005 to 2010, aiming to increase the efficiency in power generation and distribution, and to reduce the vulnerability on climate events. However, environmental impacts related to this technology, especially those impacts on human health, require a detailed analysis, considering that many DPSs have been located nearby densely populated areas. This paper presents an analysis of the external effects related to gaseous emissions from decentralized power generation in Santa Clara City, Cuba. Also a perturbation analysis aiming to reduce such effects is presented. For this purpose a rather novel method called integrated assessment of energy supply (IAES) was developed. The IAES is built on the impact pathway approach and the system perturbation analysis, but including additional developments. The first of these concerns is the implementation of a perturbations analysis to evaluate the external effects variation related to modifications in facility characteristics and operating conditions. This covers fuel type, efficiency, stacks geometry and microlocalization. Second, the exposure to polluting gases in the study area is determined taking into account the dispersion of pollutants, and the geographical distribution of the population. The exposure modelling is determinant to estimate human health impact. In this way it was found that north-west DPS cause the highest local impact on human health. This is associated with the pollutants concentration increase in densely populated areas. The higher CO_2 emissions correspond to the southeast DPS by a factor of 1.8 compared to the north-west DPS. However, the local impact related to the southeast DPS is lower, due to its location where downwind population is lower. A reduction potential on health impact of about 20% and 9% respectively was finally determined for north-west and south-west DPS.

14/02268 Feedstock specific environmental risk levels related to biomass extraction for energy from boreal and temperate forests

Lamers, P. *et al. Biomass and Bioenergy*, 2013, 55, 212–226.

Past research on identifying potentially negative impacts of forest management activities has primarily focused on traditional forest operations. The increased use of forest biomass for energy in recent years, spurred predominantly by policy incentives for the reduction of fossil fuel use and greenhouse gas emissions, and by efforts from the forestry sector to diversify products and increase value from the forests, has again brought much attention to this issue. The implications of such practices continue to be controversially debated; predominantly the adverse impacts on soil productivity and biodiversity, and the climate change mitigation potential of forest bioenergy. Current decision making processes require comprehensive, differentiated assessments of the known and unknown factors and risk levels of potentially adverse environmental effects. This paper provides such an analysis and differentiates between the feedstock of harvesting residues, roundwood, and salvage wood. It concludes that the risks related to biomass for energy outtake are feedstock specific and vary in terms of scientific certainty. Short-term soil productivity risks are higher for residue removal. There is however little field evidence of negative long-term impacts of biomass removal on productivity in the scale predicted by modelling. Risks regarding an alteration of biodiversity are relatively equally distributed across the feedstocks. The risk of limited or absent short-term carbon benefits is highest for roundwood, but negligible for residues and salvage wood. Salvage operation impacts on soil productivity and biodiversity are a key knowledge gap. Future research should also focus on deriving regionally specific, quantitative thresholds for sustainable biomass removal.

14/02269 Is energy cropping in Europe compatible with biodiversity? – Opportunities and threats to biodiversity from land-based production of biomass for bioenergy purposes

Pedroli, B. *et al. Biomass and Bioenergy*, 2013, 55, 73–86.

Based on literature and six country studies (Belgium, Denmark, Finland, Netherlands, Sweden, Slovakia) this paper discusses the compatibility of the European Union 2020 targets for renewable energy with conservation of biodiversity. The authors conclude that increased demand for biomass for bioenergy purposes may lead to a continued conversion of valuable habitats into productive lands and to intensification, which both have negative effects on biodiversity. On the other hand, increased demand for biomass also provides opportunities for biodiversity, both within existing productive lands and in abandoned or degraded lands. Perennial crops may lead to increased diversity in crop patterns, lower input uses, and higher landscape structural diversity which may all have positive effects on biodiversity. In production forest opportunities exist to harvest primary wood residues. Removal of these forest residues under strict sustainability conditions may become economically attractive with increased biomass demand. An additional biomass potential is represented by recreation areas, roadside verges, semi-natural and natural areas and lands which have no other use because they have been abandoned, polluted or degraded. Whether effects of cropping of biomass and/or removal of biomass has positive or negative impact on biodiversity depends strongly on specific regional circumstances, the type of land and land use shifts involved and the associated management practices in general. However, it is clear that in the six countries studied certain types of biomass crops are likely to be more sustainable than others.

14/02270 Local acceptance of existing biogas plants in Switzerland

Soland, M. *et al. Energy Policy*, 2013, 61, 802–810.

After the Swiss government's decision to decommission its five nuclear power plants by 2035, energy production from wind, biomass, biogas and photovoltaic is expected to increase significantly. Due to its many aspects of a direct democracy, high levels of public acceptance are necessary if a substantial increase in new renewable energy power plants is to be achieved in Switzerland. A survey of 502 citizens living near 19 biogas plants was conducted as the basis for using structural equation modelling to measure the effects of perceived benefits, perceived costs, trust towards the plant operator, perceived smell, information received and participation options on citizens' acceptance of 'their' biogas plant. Results show that local acceptance towards existing biogas power plants is relatively high in Switzerland. Perceived benefits and costs as well as trust towards the plant operator are highly correlated and have a significant effect on local acceptance. While smell perception and information received had a significant effect on local acceptance as well, no such effect was found for participation options. Reasons for the non-impact of participation options on local acceptance are discussed, and pathways for future research are presented.

14/02271 Mineral speciation and fate of some hazardous contaminants in coal waste pile from anthracite mining in Portugal

Ribeiro, J. *et al. International Journal of Coal Geology*, 2013, 109–110, 15–23.

The coal (anthracite A) in Douro coalfield (north-west Portugal) has been exploited for many years and has been mainly used as fuel supply by a thermal power plant. The mining activities inevitably impacted the environment, which includes a large number of coal waste piles emplaced over the old mine sites and adjacent areas of the Douro coalfield. The disposal of coal-mining residues represents significant environmental concerns due to their potential influence on soils and sediments, as well as on the surface and groundwater of the surrounding areas. In the present study, the development of sequential extraction combined with various advanced analytical techniques was performed to provide an improved understanding of the complex processes related with sulfide-rich coal waste oxidation, sequences of mineral formation, and the transport mechanisms of hazardous elements by specific neoformed soluble minerals. The results showed the presence of amorphous iron (oxy-) hydroxides and goethite with various degrees of crystallinity, containing hazardous elements, such as As, Cr, Hg, Mo, Se, Pb, U, and others. Some of the neoformed minerals found in the coal waste material are the same as those commonly associated with coal acid drainage, in which oxidation of sulfides plays an important role. The precipitated neoformed minerals include pickeringite, blödite, and a mixture of epsomite, pickeringite and hexahydrite. As these sulfates may dissolve after the first rain, they may release above-mentioned elements into surrounding water bodies.

14/02272 Renewable energy and unemployment: a general equilibrium analysis

Rivers, N. *Resource and Energy Economics*, 2013, 35, (4), 467–485.

Using a three-sector general equilibrium model, the impact of renewable electricity support policies on the rate of equilibrium unemployment is analysed. In a simple two-factor version of the model, the paper shows analytically that renewable electricity support policies lead to an increase in the rate of unemployment. A numerical analysis is conducted with an expanded three-factor model. In this version, most scenarios analysed also lead to an increase in equilibrium unemployment. However, the paper identifies conditions in which renewable energy support policies can decrease the rate of equilibrium unemployment. In particular, when the elasticity of substitution between capital and labour is low, when capital is not mobile internationally, and when the labour intensity of renewable generation is high relative to conventional generation, renewable electricity support policies may reduce the rate of equilibrium unemployment. The model is parameterized to represent the US economy, such that the magnitudes of quantities can be observed. Although there is some variation in the results depending on parameters, the findings suggest in general that reducing electricity sector emissions by 10% through renewable electricity support policies is likely to increase the equilibrium unemployment rate by about 0.1–0.3 percentage points.

14/02273 Spatiotemporal risk assessment of soil pollution in a lignite mining region using a Bayesian maximum entropy (BME) approach

Modis, K. *et al. International Journal of Coal Geology*, 2013, 112, 173–179.

The present paper aims to map pollution and assess the risk for agricultural soils in a wider lignite opencast mining and industrial area. Geochemical data related to environmental studies show that the waste characteristics favour solubilization and mobilization of inorganic contaminants and in some cases the generation of acidic leachates. The spatiotemporal distribution of soil contamination is studied by the application of the Bayesian maximum entropy theory which allows merging spatial and temporal estimations in a single model. Results reveal a correlation range of contaminant concentrations up to 5000 m and indicate a potential forecasting range up to 4 years. Inspection of the produced spatiotemporal maps indicates that the whole study area is contaminated by As and various heavy metals, a situation which seems to be more or less stable over time.

14/02274 The effect of urbanization on CO_2 emissions in emerging economies

Sadorsky, P. *Energy Economics*, 2014, 41, 147–153.

The theories of ecological modernization and urban environmental transition both recognize that urbanization can have positive and negative impacts on the natural environment with the net effect being hard to determine *a priori*. This study uses recently developed panel regression techniques that allow for heterogeneous slope coefficients and cross-section dependence to model the impact that urbanization has on CO_2 emissions for a panel of emerging economies. The estimated contemporaneous coefficients on the energy intensity and affluence variables are positive, statistically significant and fairly similar across different estimation techniques. By comparison, the estimated contemporaneous coefficient on the urbanization variable is sensitive to the estimation technique. In most specifications, the estimated coefficient on the urbanization variable is positive but statistically insignificant. The implications of these results for sustainable development policy are discussed.

14/02275 When energy storage reduces social welfare

Sioshansi, R. *Energy Economics*, 2014, 41, 106–116.

This paper examines the potential welfare effects of storage under different market structures. This includes combinations of perfectly competitive and strategic generation and storage sectors, and standalone and generator-owned storage. Here, the authors demonstrate that if the generation sector is perfectly competitive and does not own storage, then storage cannot be welfare diminishing. Otherwise, generator-owned storage or standalone storage in a market with strategic generating firms can reduce welfare compared to the no-storage case. This contradicts conventional wisdom that adding firms to an imperfectly competitive market typically reduces welfare losses.

14/02276 Wind farm struggles in Flanders fields: a sociological perspective

Pepermans, Y. and Loots, I. *Energy Policy*, 2013, 59, 321–328.

This study analyses how protests against wind farms reflect symbolic distances or alienations, typical to Flanders, Belgium, as consequences of wider societal trends. A thorough qualitative study of three wind farm projects in Flanders, including group discussions and interviews with crucial stakeholders, shows that the current siting process reinforces disagreements and leads to a stalemate between different framings of the wind farms. Using insights from the case studies and literature, the authors argue for spatial planning which strives for a negotiation over acceptable solutions rather than acceptance of fixed proposals.

CO_2, NO_x, SO_2 and particulate emissions

14/02277 Applying UV cameras for SO_2 detection to distant or optically thick volcanic plumes

Kern, C. *et al. Journal of Volcanology and Geothermal Research*, 2013, 262, 80–89.

Ultraviolet (UV) camera systems represent an exciting new technology for measuring two-dimensional sulfur dioxide (SO_2) distributions in volcanic plumes. The high frame rate of the cameras allows the retrieval of SO_2 emission rates at time scales of 1 Hz or higher, thus allowing the investigation of high-frequency signals and making integrated and comparative studies with other high-data-rate volcano monitoring techniques possible. One drawback of the technique, however, is the limited spectral information recorded by the imaging systems. Here, a framework for simulating the sensitivity of UV cameras to various SO_2 distributions is introduced. Both the wavelength-dependent transmittance of the optical imaging system and the radiative transfer in the atmosphere are modelled. The framework is then applied to study the behaviour of different optical setups and used to simulate the response of these instruments to volcanic plumes containing varying SO_2 and aerosol abundances located at various distances from the sensor. Results show that UV radiative transfer in and around distant and/or optically thick plumes typically leads to a lower sensitivity to SO_2 than expected when assuming a standard Beer–Lambert absorption model. Furthermore, camera response is often non-linear in SO_2 and dependent on distance to the plume and plume aerosol optical thickness and single scatter albedo. The model results are compared with camera measurements made at Kilauea Volcano (Hawaii) and a method for integrating moderate resolution differential optical absorption spectroscopy data with UV imagery to retrieve improved SO_2 column densities is discussed.

14/02278 Capturing CO_2 in flue gas from fossil fuel-fired power plants using dry regenerable alkali metal-based sorbent

Zhao, C. *et al. Progress in Energy and Combustion Science*, 2013, 39, (6), 515–534.

Carbon dioxide capture and storage (CCS) has received significant attention recently and is recognized as an important option for reducing CO_2 emissions from fossil fuel combustion. A particularly promising option involves the use of dry alkali metal-based sorbents to capture CO_2 from flue gas. Here, alkali metal carbonates are used to capture CO_2 in the presence of H_2O to form either sodium or potassium bicarbonate at temperatures below 100 °C. A moderate temperature swing of 120–200 °C then causes the bicarbonate to decompose and release a mixture of CO_2/H_2O that can be converted into a 'sequestration-ready' CO_2 stream by condensing the steam. This process can be readily used for retrofitting existing facilities and easily integrated with new power generation facilities. It is ideally suited for coal-fired power plants incorporating wet flue gas desulfurization, due to the associated cooling and saturation of the flue gas. It is expected to be both cost-effective and energy efficient. This paper provides the first comprehensive review of the major research progress on this technology. To date such research has focused on two main areas: sorbent development and process development. In the case of sorbent development, pure sodium carbonate and potassium carbonate were tested directly. More recent research has concentrated on using supported sorbents which provide the necessary attrition resistance for use with fluidized-bed or transport reactors. Research on sorbent development has included an examination of the physical properties, carbonation and regeneration reaction behaviour, reaction kinetic behaviour, and multi-cycle behaviour of these alkali metal-based sorbents. By contrast, process development activities have focused on solving the many unique challenges associated with post-combustion CO_2 capture using alkali metal-based sorbents. The research on process development included exploration of the effects of operation conditions such as reaction temperature, gas composition, operation pressure, and gas impurities on CO_2 capture behaviour, continuous operation of the CO_2 capture process, and economic evaluation of this process. Finally, this paper discusses the research challenges and opportunities that exist with this technology.

14/02279 Comparison of solvent performance for CO_2 capture from coal-derived flue gas: a pilot scale study

Frimpong, R. A. *et al. Chemical Engineering Research and Design*, 2013, 91, (6), 963–969.

The performance of a proprietary solvent (CAER-B2), an amine–carbonate blend, for the absorption of CO_2 from coal-derived flue gas is evaluated and compared with state-of-the-art 30 wt% monoethanolamine (MEA) under similar experimental conditions in a 0.1 MWth pilot plant. The evaluation was done by comparing the carbon capture efficiency, the overall mass transfer rates, and the energy of regeneration of the solvents. For similar carbon loadings of the solvents in the scrubber, comparable mass transfer rates were obtained. The rich loading obtained for the blend was 0.50 mol CO_2/mol amine compared to 0.44 mol CO_2/mol amine for MEA. The energy of regeneration for the blend was about 10% lower than that of 30 wt% MEA. At optimum conditions, the blend shows promise in reducing the energy penalty associated with using industry standard, MEA, as a solvent for CO_2 capture.

14/02280 CO_2 emissions from household consumption in India between 1993–94 and 2006–07: a decomposition analysis

Das, A. and Paul, S. K. *Energy Economics*, 2014, 41, 90–105.

Carbon dioxide emissions from anthropogenic activities are considered to be one of the major causes of global warming. In India, being an agriculture-dependent country, global warming would mean monsoon instability and consequent food scarcity, natural disasters and economic concerns. However, with proper policy interventions, CO_2 emissions can be controlled. Input–output analysis has been used to estimate direct and indirect CO_2 emissions by households for 1993–1994, 1998–1999, 2003–2004 and 2006–2007. Complete decomposition analysis of the changes in CO_2 emissions between 1993–1994 and 2006–2007 has been done to identify the causes into pollution, energy intensity, structure, activity and population effects according to broad household consumption categories. Results indicate that activity, structure and population effects are the main causes of increase in CO_2 emissions from household fuel consumption. To identify the causes at the sectoral level, a second decomposition has been done for changes between 2003–2004 and 2006–2007 to identify the causes in the next stage. Finally, alternative energy policy options have been examined for each consumption category to reduce emissions. Combined strategies of technology upgrading, fuel switching and market management in order to reduce CO_2 emissions for sectors such as batteries, other non-electrical machinery, construction and electronic equipment (including televisions), for which all the effects are positive, need to be adopted.

14/02281 Design of carrier-based offshore CCS system: plant location and fleet assignment

Nam, H. *et al. International Journal of Greenhouse Gas Control*, 2013, 12, 220–230.

As part of efforts to mitigate the global effects of greenhouse gases from fossil fuels, CO_2 capture and storage (CCS) technology has drawn large attention from the engineering research community. Compared to a pipeline-based system, an offshore CCS system using liquefied CO_2 (LCO_2) carrier ships and offshore oil wells is expected to offer a more flexible and efficient mode of CCS to many countries, especially nations such as Korea where a pipeline-based system is inherently infeasible. In this paper, the authors discuss a carrier-based offshore CCS system, in which CO_2 carriers may transport crude oils on inbound voyage, and seek the optimal configuration of the system including liquefaction plant location, fleet assignment and the optimal pressure and temperature of the cargo CO_2. The authors determined the optimal system configuration including the liquefaction plant location and CO_2 carrier fleet assignment with respect to the overall transport cost of the CCS system. They used two sequential linear programming problems: plant location and fleet assignment, with the pressure and temperature state of cargo CO_2 as the key CCS chain parameters. The optimal state of CO_2 at each stage in the system was found to deviate from the triple point, depending on the system's configuration and throughput. As a case study, the study demonstrated that the optimal cargo state can be different from the triple point depending on the system configuration. In this case it is −39 °C and 10 bar and the overall transport cost of CO_2 sequestration is US$26.7/ton. This result was based on the specific scenario of the CO_2 capture and storage system for Korea using southeastern Asian offshore oil wells.

14/02282 Experimental simulation of the impact of a thermal gradient during geological sequestration of CO_2: the COTAGES experiment

Jobard, E. *et al. International Journal of Greenhouse Gas Control*, 2013, 12, 56–71.

This study investigated the reactivity of crushed oolithic limestone that is exposed to high-pressure CO_2 and a high thermal gradient (100–35 °C in a 78 cm long tubular reactor) for 30 days. The original COTAGES experiment described in this paper was carried out in the presence of saline aqueous solution (4 g L^{-1} NaCl) at equilibrium with $CaCO_3$ at 100 °C. Mass transfer was observed from the cold area of the reactor (35–55 °C) to the warmest area (100 °C) and constituted approximately 10% of the initial mass of the most reactive sample, suggesting the presence of calcite dissolution and precipitation. Petrographical analyses using electronic and cathodoluminescence microscopes and X-ray microtomography showed that the dissolution mainly affected the cortices of ooliths located in the periphery of the grains and created more than 700 pore mm^{-2} in the most reactive sample. However, because of their small sizes (mostly less than 100 μm^2), the pores did not significantly increase the porosity (2% on average). The crystallization of a microcalcite fringe in the warmed area covered the entire surface of the grains and isolated the porous network of grains in a sample. This study demonstrates the strong reactivity of oolithic limestone in the presence of a thermal gradient and pressure similar to realistic CO_2 geological sequestration conditions with mass transport from the injection well towards the reservoir rock.

14/02283 Fluid bed adsorption of carbon dioxide on immobilized polyethylenimine (PEI): kinetic analysis and breakthrough behavior

Monazam, E. R. *et al. Chemical Engineering Journal*, 2013, 223, 795–805.

The adsorption of carbon dioxide (CO_2) by immobilized polyethylenimine (PEI) on mesoporous silica was investigated in a fluid bed. The tests were performed to determine breakthrough behaviour with varying bed temperature, flow rates and feed concentrations. Experimental breakthrough curves were analysed using a theoretical one-dimensional model developed by Bohart and Adams. The results showed that Bohart–Adams model was suitable for the normal description of breakthrough curve for the temperature ranges of 40–90 °C. The maximum capacity increased with temperature up to 70 °C and then decreased. The adsorption rate constant exhibited a negative temperature dependence decreasing as the temperature increased. Parameters characteristic of a fluid bed adsorber were inferred from these breakthrough curves including the breakthrough time, saturation time, critical reactor length, and length of mass transfer zone. These parameters can be used to design fluid bed adsorption system without resolving the mechanistic contributions of dispersion, mixing, and intraparticle diffusion.

14/02284 Influence of EGR and oxygen-enriched air on diesel engine NO–smoke emission and combustion characteristic

Zhang, W. *et al. Applied Energy*, 2013, 107, 304–314.

The oxygen-enriched combustion of diesel engines can reduce smoke emission and increase engine thermal efficiency; however it can also lead to an increase of NO emission. In this paper, an experiment was conducted on a turbocharged direct injection diesel engine, and oxygen-enriched and exhaust gas recirculation (EGR) techniques were used to produce lower NO–smoke emission than the unmodified engine under the same fuel supply rate curve and fuel supply quantity. The specific fuel consumption and the power loss were lower than 5% compared to the unmodified engine. The effect of oxygen enrichment on the particle size distribution was tested and analysed. The results revealed that the optimal NO–smoke emission can be achieved at these conditions: 1600 rpm of engine speed, full load, 30–40% EGR rate and 21.5–22.5% of intake oxygen density; 2200 rpm of engine speed, full load, 20–45% EGR rate and 22–24% of intake oxygen density. The result of particle size distribution tests revealed that oxygen enriched combustion can effectively suppress the diameter growth of particles and lead to fewer large particles with a diameter larger than 100 nm emissions; however it did lead to an increase of 15 nm small particles. A reduced n-heptane kinetic model was also developed in this research which contained NO and polycyclic aromatic hydrocarbons (PAHs) formation mechanisms, and the model was coupled with a CFD model to simulate the oxygen-enriched combustion of a diesel engine. The calculated results demonstrated that the coupled model can accurately predict ignition time and the change of in-cylinder pressure when the combined oxygen-enriched and EGR technique was used. The computed NO change with in-cylinder oxygen density agreed well with experiment results, and the computed result of the growth experience of PAHs showed that oxygen-enriched combustion can effectively suppress the hydrogen abstraction C_2H_2 addition reaction during PAHs formation, which leads to the reduction of large molecule PAHs, and this result agreed well with the observed situation that particle size diameter decreases with the increase of intake oxygen density.

14/02285 Involvement of water and visible light in the enhancement in SO_2 adsorption at ambient conditions on the surface of zinc (hydr)oxide/graphite oxide composites

Seredych, M. *et al. Chemical Engineering Journal*, 2013, 223, 442–453.

Composites of zinc (hydr)oxide–graphite oxide and of zinc (hydr)oxide–graphene were used as adsorbents of sulfur dioxide at ambient conditions. The initial and exhausted samples were characterized by X-ray diffraction, Fourier transform infrared spectroscopy, potentiometric titration, energy-dispersive X-ray spectroscopy, thermal analysis and adsorption of nitrogen. Cyclic voltammetry in light and dark was also used to show the photoactivity of the samples. The results obtained suggest that visible-light-enhanced water splitting reaction takes place on the surface of zinc (hydr)oxide and its composite with graphite oxide. This results in a significant improvement of these materials' performance as SO_2 adsorbents at ambient conditions. Owing to the presence of electrons–hole pairs and their spatial separation by a conductive graphene based phase, at one location SO_2 accepts the electrons and sulfide and sulfur are formed, whereas at the separate locations, where holes exist, SO_2 acts as electron donor and sulfates are deposited on the surface with the release of hydrogen. Sulfur dioxide feeding to the system and running the experiments in the visible light provide the continuity to this process. The exhaustion of materials' reactive adsorption capability happens when sulfur species are deposited on all active sites, and therefore the active centres for water splitting and electron transfer are blocked and/or lose their photoactive properties.

14/02286 Modeling fuel NO_x formation from combustion of biomass-derived producer gas in a large-scale burner

Sukumaran, S. and Kong, S.-C. *Combustion and Flame*, 2013, 160, (10), 2159–2168.

This study investigates the characteristics of fuel NO_x formation resulting from the combustion of producer gas derived from biomass gasification using different feedstocks. Common industrial burners are optimized for using natural gas or coal-derived syngas. With the increasing demand in using biomass for power generation, it is important to develop burners that can mitigate fuel NO_x emissions due to the combustion of ammonia, which is the major nitrogen-containing species in biomass-derived gas. In this study, the combustion process inside the burner is modelled using computational fluid dynamics with detailed chemistry. A reduced mechanism (36 species and 198 reactions) is developed from GRI 3.0 in order to reduce the computation time. Combustion simulations are performed for producer gas arising from different feedstocks such as wood gas, wood + 13% DDGS (dried distiller grain soluble) gas and wood + 40% DDGS gas and also at different air equivalence ratios ranging from 1.2 to 2.5. The predicted NO_x emissions are compared with the experimental data and good levels of agreement are obtained. It is found out that NO_x is very sensitive to the ammonia content in the producer gas. Results show that although NO–NO_2 interchanges are the most prominent reactions involving NO, the major NO producing reactions are the oxidation of NH and N at slightly fuel rich conditions and high temperature. Further analysis of results is conducted to determine the conditions favourable for NO_x reduction. The results indicate that NO_x can be reduced by designing combustion conditions which have fuel rich zones in most of the regions. The results of this study can be used to design low NO_x burners for combustion of gas mixtures derived from gasification of biomass. One suggestion to reduce NO_x is to produce a diverging flame using a bluff body in the flame region such that NO generated upstream will pass through the fuel rich flame and be reduced.

14/02287 Numerical prediction of CO_2 capture process by a single droplet in alkaline spray

Chen, W.-H. *et al. Applied Energy*, 2013, 109, 125–134.

Carbon dioxide captured by single droplets in sprays plays a fundamental role in reducing greenhouse gas emissions. This study focuses on CO_2 capture processes in single droplets in alkaline sprays using a numerical method. Three different initial pH values of 10, 11, and 12 in the droplet are considered. The capture behaviour in the absence of chemical dissociation is also investigated for comparison. The predictions suggest that the chemical dissociation in the droplet substantially elongates the CO_2 capture process and the mass diffusion is the controlling mechanism of CO_2 capture process. For the chemical absorption, the final CO_2 capture amount by the droplet is mainly determined by HCO_3^- which is significantly influenced by the initial pH value. An increase in initial pH value raises the carbon capture amount by the droplet. The mean concentration of CO_3^{2-} is highly related to the variation of mean pH value, but its concentration is by far lower than those of $H_2O \cdot CO_2$ and HCO_3^-. Corresponding to the initial pH values of 10, 11, and 12, the times required for turning the basic droplet to the acidic one are in the orders of 10, 100 and 1000 ms. On account of larger carbon capture amount and shorter absorption period at a higher initial pH value, the carbon capture rate is lifted as the initial pH value rises, and CO_2 capture by droplets at the initial pH value of 12 is better than those at 10 and 11.

14/02288 Optimisation-oriented modelling of the NO_x emissions of a Diesel engine

Asprion, J. *et al. Energy Conversion and Management*, 2013, 75, 61–73.

Model-based optimization is gaining more and more ground in automotive engineering. The underlying models have to be smooth, fast, quantitatively accurate, and need to provide plausible extrapolation. A previously published model for the NO_x emissions of a Diesel engine incorporates all these requirements but relies on the measured in-cylinder pressure. In this paper, that model is embedded in a mean-value model for the air path. Thus, the NO_x emissions can be predicted based on the control signals only. Physics-based models are developed for the interfacing processes such as the cylinder charge, its composition, the compression, and the ignition delay. The accuracy of the original model is preserved, while the execution time of the extended NO_x model is found to be only a fraction of that of the mean-value engine model. An experimental validation on an actual transient driving cycle highlights the advantages of the procedure presented.

14/02289 Self-activation and effect of regeneration conditions in CO_2–carbonate looping with CaO–$Ca_{12}Al_{14}O_{33}$ sorbent

Stendardo, S. *et al. Chemical Engineering Journal*, 2013, 220, 383–394.

Carbon dioxide capture by solid sorbents through uptake–regeneration cycling is a promising option for high temperature removal of CO_2 from combustion gases and synthesis/fuel gases. The present study investigates the influence of regeneration atmosphere and temperature on the CO_2 uptake capacity during repeated cycling of CaO-based solid sorbents. The sorbents were synthesized to contain 75 and 85% w/w of active phase (CaO) and binder ($Ca_{12}Al_{14}O_{33}$) and were then subjected to cycling tests with repeated CO_2 uptake and release in a thermogravimetric analyser for up to 200 cycles. Test conditions were chosen to test high-temperature CO_2 capture at 600 °C in an atmosphere containing 14 and 25% v/v CO_2 (N_2 balance). Three different regeneration conditions were tested: (a) mild condition: regeneration at 900 °C in 14% CO_2 or 100% N_2; (b) moderate condition: regeneration at 1000 °C in 14% CO_2 and (c) severe condition: regeneration at 1000 °C in 86% CO_2. Hydration of the sorbent during synthesis and prolonged carbonation prior to the cycling tests significantly improved the stability of the uptake capacity. Interestingly, the pretreated 75% w/w CaO synthetic sorbent maintained a good uptake capacity up to the 150th cycle under severe regeneration conditions and even showed continuously increasing CO_2 uptake capacity throughout the 150-cycle test with 25% CO_2. The 75% w/w CaO sorbent is thus an interesting candidate for future work on high-temperature CO_2 capture.

14/02290 Simultaneous carbon and nitrogen removals in membrane bioreactor with mesh filter: an experimental and modeling approach

Wang, Y.-K. *et al. Chemical Engineering Science*, 2013, 95, 78–84.

In this study, an intermittently aerated membrane bioreactors (MBR) with stainless-steel mesh as a filter was developed for simultaneous effective carbon and nitrogen removals. The biofilm attached on mesh filter can effectively reject suspended solids to improve effluent quality. The chemical oxygen demand (COD) and nitrogen removal efficiencies of the system were examined at different influent COD/N ratios, dissolved oxygen (DO) levels and aerobic/anoxic time ratios. The reactor achieved COD, NH_4^+–N and total nitrogen removals over 93.7%, 92.8% and 79.5%, respectively. To get a better insight into this process, a mechanistic mathematical model was developed based on the activated sludge model No. 3 (ASM3) for the process simulation. The simulation results agreed with the measured data well. The optimization results show that an appropriate DO level in the aerobic phase and a prolonged anoxic time is required to further improve the total nitrogen removal.

14/02291 Strategic route map of sulphur dioxide reduction in China

Yuan, X. *et al. Energy Policy*, 2013, 60, 844–851.

China's economy has risen to be the world's second largest since 2010, accompanied by the world's largest energy consumption. As one of the major air pollutants from the fossil fuel, excessive SO_2 emissions have severe negative impacts on eco-environments. In order to achieve the balance between economic growth and environmental protection, many efforts have been made on the reduction of SO_2. The route map for the reduction of SO_2 in China includes policy setting, economic and energy structure adjustment, and the construction of desulfurization facilities. These initiatives and efforts together had resulted in the significant reduction of SO_2 emissions along with fast economic development. This study provides a useful reference for other developing countries in coping SO_2 control. The findings also provide implications for reducing the other two air pollutants with binding control targets in the twelfth Five-Year Plan period in China, i.e. NO_x and CO_2.

14/02292 Technology roadmap study on carbon capture, utilization and storage in China
Zhang, X. *et al. Energy Policy*, 2013, 59, 536–550.
Carbon capture, utilization and storage (CCUS) technology will likely become an important approach to reduce CO_2 emissions and optimize the structure of energy consumption in China in the future. In order to provide guidance and recommendations for CCUS research, development and demonstration in China, a high-level stakeholder workshop was held in Chongqing in June 2011 to develop a technology roadmap for the development of CCUS technology. This roadmap outlines the overall vision to provide technically viable and economically affordable technological options to combat climate change and facilitate socio-economic development in China. Based on this vision, milestone goals from 2010 to 2030 are set out in accordance with the technology development environment and current status in China. This study identifies the critical technologies in capture, transport, utilization and storage of CO_2 and proposes technical priorities in the different stages of each technical aspect by evaluating indices such as the objective contribution rate and technical maturity, and gives recommendations on deployment of full-chain CCUS demonstration projects. Policies which would support CCUS are also suggested in this study.

Hydrocarbon emissions

14/02293 A study of nitrogen conversion and polycyclic aromatic hydrocarbon (PAH) emissions during hydrochar–lignite co-pyrolysis
Liu, Z. *et al. Applied Energy*, 2013, 108, 74–81.
Nitrogen conversion and polycyclic aromatic hydrocarbon (PAH) formation during rapid pyrolysis of hydrochar, lignite and hydrochar–lignite blends have been investigated within a temperature range of 600–900 °C. The results showed that in comparison to lignite, a higher percentage of hydrochar nitrogen was retained in the char, and less NH_3 and HCN were formed during pyrolysis. During pyrolysis of the individual hydrochar and lignite components, yields of NH_3 and HCN reached a maximum at 800 °C and then decreased with increasing temperature. Addition of hydrochar to the lignite increased yields of total HCN and NH_3 at low pyrolysis temperatures ($\leq$700 °C), but suppressed their formation at high temperatures ($\geq$800 °C). Synergistic interactions in hydrochar–lignite blends significantly decreased the total nitrogen percentage in the char, and promoted the conversion into N_2 at temperatures $\geq$800 °C. These synergistic interactions increased with (but were not linearly proportional to) increasing temperatures and hydrochar ratios in the blends. With regard to PAH emissions, relatively less high-ring PAHs were present in tars from pyrolysis of hydrochar–lignite blends than in tars from pyrolysis of lignite alone. These findings suggest that co-processing of hydrochar–lignite blends for energy production may have the additional benefit of reducing emissions of nitrogen pollutants and PAHs.

14/02294 Emission and size distribution of particle-bound polycyclic aromatic hydrocarbons from residential wood combustion in rural China
Shen, G. *et al. Biomass and Bioenergy*, 2013, 55, 141–147.
Emissions and size distributions of 28 particle-bound polycyclic aromatic hydrocarbons (PAHs) from residential combustion of 19 fuels in a domestic cooking stove in rural China were studied. Measured emission factors of total particle-bound PAHs were 1.79 ± 1.55, 12.1 ± 9.1 and $5.36 \pm 4.46\,mg\,kg^{-1}$ for fuel wood, brushwood and bamboo, respectively. Approximately 86.7%, 65.0% and 79.7% of the PAHs were associated with fine particulate matter with size less than 2.1 μm for these three types of fuels, respectively. Statistically significant differences in emission factors and size distributions of particle-bound PAHs between fuel wood and brushwood were observed, with the former had lower emission factors but more PAHs in finer particulate matter. The mass fraction of the fine particles associated with PAHs was found to be positively correlated with fuel density and moisture, and negatively correlated with combustion efficiency. Low and high molecular weight PAHs preferably segregated into the coarse and fine particulate matter, respectively. The high accumulation tendency of the PAHs from residential wood combustion in fine particles implies strong adverse health impact.

14/02295 Investigation on the solidification of several pure cyclic and aromatic hydrocarbons at pressures to 300 MPa
Wu, Y. *et al. Fuel*, 2013, 111, 75–80.
The effect of pressure on the solidification of several saturated cyclic hydrocarbons and three xylene isomers are experimentally determined with a variable-volume view cell at pressures to 300 MPa and temperatures starting at 293.15 K. Solid–liquid transitions are observed for cyclooctane, *cis*-1,2-dimethylcyclohexane, *trans*-1,4-dimethylcyclohexane, *p*-xylene, *o*-xylene, and 2-methylnaphthalene. However, methylcyclohexane, ethylcyclohexane, *cis*-1,4-dimethylcyclohexane, and *m*-xylene remained liquid over the same operating pressure and temperature ranges. The experimental solid–liquid transition data are well represented with two empirical equations, the Simon equation and a second-order polynomial equation. Data obtained in this study agree with literature results within ±0.4% for 2-methylnaphthalene and ±0.2% for *p*-xylene.

14/02296 Machine learning models for predicting PAHs bioavailability in compost amended soils
Wu, G. *et al. Chemical Engineering Journal*, 2013, 223, 747–754.
Compost addition to polluted soils is a strategy for waste reuse and soil remediation, while bioavailability is a key parameter for environmental assessment. Empirical data from an 8-month microcosm experiment were used to assess the ability and performance of six machine learning (ML) models to predict temporal bioavailability changes of 16 polycyclic aromatic hydrocarbons (PAHs) in contaminated soils amended with compost. The models included multilayer perceptrons (MLPs), radial basis function (RBF), support vector regression (SVR), M5 model tree (M5P), M5 rule (M5R) and linear regression (LR). Overall, the performance of the six models, determined by 10-fold cross-validation method, was ranked as follows: RBF > M5P > SVR > MLP > M5R > LR. Results further demonstrated that the ML models successfully identified the relative importance of each variable (i.e. incubation time, organic carbon content, soil moisture content, nutrient levels) on the temporal bioavailability change of individual PAH. Such models can potentially be useful for predicting the concentration of a wide range of pollutants in soils, which could contribute to reduce chemical monitoring at site and help decision making for remediation end points and risk assessment.

Life cycle analysis

14/02297 A life cycle assessment of pennycress (*Thlaspi arvense L.*)-derived jet fuel and diesel
Fan, J. *et al. Biomass and Bioenergy*, 2013, 55, 87–100.
Field pennycress (*Thlaspi arvense L.*) is a member of the mustard family and may be grown as a winter crop between traditional summer crops to produce renewable biomass for renewable diesel and jet fuel. This paper estimated total annual biofuel production potential of 15 million cubic metres from rotation between corn and soybeans on 16.2 million hectares in the US Midwest without impact on food production. This study also investigated the life cycle greenhouse gas (GHG) emissions and energy balance of pennycress-derived hydro-processed renewable jet (HRJ) fuel and renewable diesel (RD). Both system expansion and allocation approaches were applied to distribute environmental impacts among products and co-products along the life cycle of each biofuel. The life cycle GHG emissions (excluding land use change) for RD and HRJ range from 13 to $41\,g\,MJ^{-1}$ (CO_2 eq.) and -18 to $45\,g\,MJ^{-1}$ (CO_2 eq.), respectively, depending on how the co-products are credited. The majority of the energy required for each biofuel product is derived from renewable biomass as opposed to non-renewable fossil. The fossil energy consumptions are considerably lower than the petroleum fuels. Scenario analyses were also conducted to determine response to model assumptions, including nitrogen fertilizer application rate, nitrogen content in crop residues, and sources of H_2. The results show that pennycress-derived biofuels could qualify as advanced biofuels and as biomass-based diesel as defined by the Renewable Fuels Standard (RFS2).

14/02298 A systematic methodology for the environomic design and synthesis of energy systems combining process integration, life cycle assessment and industrial ecology
Gerber, L. *et al. Computers & Chemical Engineering*, 2013, 59, 2–16.
This paper presents a systematic methodology for sustainable process systems design, combining the principles of industrial ecology, process design and process integration, life cycle assessment and multi-objective optimization. The superstructure considers an extended decision perimeter and embeds models based either on flowsheeting software or average market technologies, for which energy and material flows are extracted from the life cycle inventory database. Therefore, the overall supply chain can be synthesized within a given action system and the systematic recyclings identified. The methodology can be used to design eco-industrial parks or urban systems, to identify the best conversion pathways of resources or waste, or to fix the optimal value of environmental taxes. It is illustrated by an application to the environomic design of an urban energy system. This case study considers multiple energy services to be supplied and waste to be treated, with their seasonal variations, indigenous and imported resources, as well as different candidate conversion technologies.

Results demonstrate that integrating an environmental objective in the design procedure leads to consider different system configurations than if only economic aspects are considered. The problematic of the optimal value of a CO_2 tax is as well addressed.

14/02299 Development of electric vehicles use in China: a study from the perspective of life-cycle energy consumption and greenhouse gas emissions
Zhou, G. *et al. Energy Policy*, 2013, 59, 875–884.
China has promoted the use of electric vehicles vigorously since 2009; the programme is still in its pilot phase. This study investigates the development of electric vehicle use in China from the perspectives of energy consumption and greenhouse gas (GHG) emissions. Energy consumption and GHG emissions of plug-in hybrid electric vehicles (PHEVs) and pure battery electric vehicles (BEVs) are examined on the level of the regional power grid in 2009 through comparison with the energy consumption and GHG emissions of conventional gasoline internal combustion engine vehicles. The life-cycle analysis module in Tsinghua-LCAM, which is based on the GREET platform, is adopted and adapted to the life-cycle analysis of automotive energy pathways in China. Moreover, medium- (2015) and long-term (2020) energy consumption and GHG emissions of PHEVs and BEVs are projected, in accordance with the expected development target in the Energy Efficient and Alternative Energy Vehicles Industry Development Plan (2012–2020) for China. Finally, policy recommendations are provided for the proper development of electric vehicle use in China.

14/02300 Evaluation of the environmental impact of experimental buildings with different constructive systems using material flow analysis and life cycle assessment
Rincón, L. *et al. Applied Energy*, 2013, 109, 544–552.
Sustainability of building construction systems depends on their material and energy consumption, and the consequent environmental impact. Thus, the evaluation of their sustainability requires a wide analysis that includes these three topics. Material flow analysis (MFA) and life cycle assessment (LCA) used together can offer a full environmental evaluation. For this reason, in this study, five different facade constructive systems are evaluated with MFA and LCA to compare them from an environmental point of view. The constructive systems were monitored in an experimental set-up located in Mediterranean continental climate, registering energy consumptions for summer and winter periods. MFA evaluated their total material requirement and the ecological rucksack. LCA evaluated their impact on the environment. The energy parameter considered the embodied energy of the materials and the energy consumption registered in the experimental set-up. MFA results show the significant quantity of natural resource extraction required for building which leads to a considerable ecological rucksack. On the other hand, LCA results show the importance of the operational phase of the building in the overall building energy consumption, and therefore in the environmental impact.

14/02301 Life cycle analysis in the construction sector: guiding the optimization of conventional Italian buildings
Asdrubali, F. *et al. Energy and Buildings*, 2013, 64, 73–89.
Life cycle assessment (LCA) is a widely known methodology for 'cradle to grave' investigation of the environmental impacts of products and technological lifecycles; however, this methodology has not been yet broadly used as an eco-design tool among the practitioners of the building sector. The authors applied LCA on three conventional Italian buildings: a detached residential house, a multi-family and a multi-storey office building. The analysis includes all the life stages, from the production of the construction materials, to their transportation, assembling, lighting, appliances, cooling- and heating-usages during the operating phase, to the end of life of all the materials and components. The authors found that the operation phase has the greatest contribution to the total impact (from 77% of that of the detached house, up to 85% of the office building), whereas the impact of the construction phase ranges from about 14% (office building) to 21% (detached house). They carried further analyses to evaluate the influence of various optimizations of the buildings, e.g. more efficient envelopes and facilities, on the entire life cycle of the three buildings. In addition, the authors propose a methodological approach, which can contribute to the acceptance of LCA as a tool in the eco-friendly design of buildings, especially those buildings whose impact during the construction phase needs to be carefully checked, such as nearly zero-energy buildings.

14/02302 Life cycle assessment of a passive house in a seismic temperate zone
Proietti, S. *et al. Energy and Buildings*, 2013, 64, 463–472.
This paper presents the results of a detailed life cycle assessment (LCA) study of a low-energy consumption building (thermal energy for heating equal to 11 kWh/m^2 year) located in Perugia, Italy, according to European ISO 14040 and 14044. The building matches the criteria of environmental sustainability and bio-architecture, complying with the 'PassivHaus' standard. All life cycle phases were included in the research: acquisition and production of materials, on-site construction and use/maintenance, demolition and material disposal (100% land-filling and demolition with waste recycling). A life span of 70 years was considered. The research was therefore focused on cradle-to-grave life, based on data collected by authors, integrated with data from the literature. In particular the study was carried out to analyse the following: the benefits due to the use of recycled materials, a solar photovoltaic (during the utilization years) and the final demolition of the building. The LCA modelling was performed using the SimaPro software application, connected to the ecoinvent database. The results show that applying energy saving measures (highly insulated building envelope and passive-house standard, solar photovoltaic, waste recycling and recycled products in pre-production phase) could significantly decrease the impact of modern dwellings, with the consciousness that new ways of building do not always provide a positive environmental outcome.

14/02303 Life cycle assessment of carbon capture and storage in power generation and industry in Europe
Volkart, K. *et al. International Journal of Greenhouse Gas Control*, 2013, 16, 91–106.
To prevent serious negative effects of climate change, greenhouse gas (GHG) emission reductions are required on global level and at large scale. One option is carbon capture and storage (CCS) which aims to capture carbon dioxide (CO_2) emissions from power generation and industry and store it permanently in geologic structures. For a comprehensive comparative assessment of the environmental performance of CCS technologies life cycle assessment (LCA) is required. This study provides a systematic comparison of LCA-based environmental performances of fossil and wood power plants as well as cement production in Europe for 2025 and 2050 with and without CCS. The implementation of CCS leads to life cycle GHG emission reductions of 68–92% for fossil power generation and 39–78% for cement production whilst to negative ones for wood power generation. There are trade-offs with respect to environmental and human health impacts due to direct (e.g. air emissions) and indirect (e.g. coal mining) impacts of the increase in fuel use and additional processes and materials necessary for CCS. Cement plants are suitable point sources for the implementation of CCS. Here the energy supply for the CO_2 capture and compression is decisive for the environmental impacts, what indicates benefits of system integration.

14/02304 Life cycle greenhouse gas emission assessment of major petroleum oil products for transport and household sectors in India
Garg, A. *et al. Energy Policy*, 2013, 58, 38–48.
Energy security concerns due to high oil import dependence and climate change concerns due to related greenhouse gas (GHG) emissions are important policy discussions in India. Could life cycle assessment (LCA) of petroleum oil products provide inputs to crude oil sourcing and domestic oil pricing policies to address the two concerns? This paper presents a baseline study on LCA of petroleum products in India from well to storage depending on the oil source, type of refinery, product and the selected destinations. The LCA-based GHG emissions are found to be higher by 4–12% than GHG emissions from direct fuel consumption alone for LPG, 7–10% for gasoline, 3–9% for diesel and 4–10% for kerosene based on various supply chain routes supplying oil to six largest cities in India. Overall, the energy used in oil exploration, refinery and transportation in the LCA have a share of 72–77%, 11–15% and 6–8%, respectively. The paper proposes imposing a relative carbon tax for various oil products in different Indian cities. States could accommodate this additional carbon tax by reducing their respective state taxes without increasing the final delivery price to the consumers.

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Supplies, policy, economics, forecasts

14/02305 A comparative study of the design and construction process of energy efficient buildings in Germany and Sweden
Schade, J. *et al. Energy Policy*, 2013, 58, 28–37.

Reducing the energy consumption of buildings is an important goal for the European Union. However, it is therefore of interest to investigate how different member states address these goals. Countries such as Sweden and Germany have developed different strategies for energy conservation within the building sector. A longitudinal comparison between implemented energy conservation key policy instruments in Sweden and Germany and a survey regarding the management of energy requirements in the building process shows the following. (1) No evidence is found that energy consumption is of great importance for producing competitive offers, either for Swedish or German clients. (2) The Swedish market-driven policy has not been as successful as the German regulation policy in decreasing the energy consumption of new buildings. (3) Building standards and regulations regarding energy performance affects how professionals are educated and the way energy requirements and demands are managed throughout the building process. In conclusion, the client's demand will govern the development of energy efficient buildings. Therefore, in order to use market-driven policies, the desired parameters must be of concern for the customer to influence the majority of building projects to be more energy efficient than is specified in national standards and regulations.

14/02306 A survey of energy policy priorities in the United States: energy supply security, economics, and the environment

Manley, D. K. *et al. Energy Policy*, 2013, 60, 687–696.

Security, environment, and economic concerns are commonly identified as three major objectives of energy policy. State and federal governments have set aggressive targets for carbon emissions reductions and for alternative fuel use and increased vehicle efficiency to reduce petroleum consumption. Moreover, jobs creation and gross domestic product growth are often cited as key drivers for energy policies. Previous studies on energy policy decision-making have examined the process for developing and evaluating options using multi-criteria decision analysis tools. In addition, energy opinion polls have either elicited preferences between two goals or whether the public supports a specific policy action. This study reports results from a survey of 884 members of professional membership organizations on how the USA should prioritize energy policy across the goals of energy supply security, environment and climate, and economics and job creation. The majority favour policymaking that is balanced across all three. Security and economic concerns increase with age for male respondents, whereas environment is the highest priority for females regardless of age. Unlike previous surveys that target the general public and focus on a particular objective or technology, these results provide an example of eliciting a portfolio allocation across multiple energy policy goals from targeted constituents.

14/02307 Carbon tax scenarios and their effects on the Irish energy sector

Di Cosmo, V. and Hyland, M. *Energy Policy*, 2013, 59, 404–414.

This study uses annual time series data from 1960 to 2008 to estimate the long run price and income elasticities underlying energy demand in Ireland. The Irish economy is divided into five sectors: residential, industrial, commercial, agricultural and transport, and separate energy demand equations are estimated for all sectors. Energy demand is broken down by fuel type, and price and income elasticities are estimated for the primary fuels in the Irish fuel mix. Using the estimated price and income elasticities, the study forecasts Irish sectoral energy demand out to 2025. The share of electricity in the Irish fuel mix is predicted to grow over time, as the share of carbon intensive fuels such as coal, oil and peat, falls. The share of electricity in total energy demand grows most in the industrial and commercial sectors, while oil remains an important fuel in the residential and transport sectors. Having estimated the baseline forecasts, two different carbon tax scenarios are imposed and the impact of these scenarios on energy demand, carbon dioxide emissions, and government revenue is assessed. If it is assumed that the level of the carbon tax will track the futures price of carbon under the European Union emission trading scheme, the carbon tax will rise from €21.50 per tonne CO_2 in 2012 (the first year forecasted) to €41 in 2025. Results show that under this scenario total emissions would be reduced by approximately 861,000 tonnes of CO_2 in 2025 relative to a zero carbon tax scenario, and that such a tax would generate €1.1 billion in revenue in the same year. The authors also examine a high tax scenario under which emissions reductions and revenue generated will be greater. Finally, in order to assess the macroeconomic effects of a carbon tax, the carbon tax scenarios were run in HERMES, the Economic and Social Research Institute's medium-term macroeconomic model. The results from HERMES show that, a carbon tax of €41 per tonne CO_2 would lead to a 0.21% contraction in gross domestic product, and a 0.08% reduction in employment. A higher carbon tax would lead to greater contractions in output.

14/02308 Centralised utility system planning for a total site heat integration network

Liew, P. Y. *et al. Computers & Chemical Engineering*, 2013, 57, 104–111.

Total site heat integration (TSHI) is a technique of exchanging heat among multiple processes via a centralized utility system. An analysis of the integrated multiple processes, also known as the total site (TS) system sensitivity, is needed to characterize the effects of a plant maintenance shutdown, to determine the operational changes needed for the utility production and to plan mitigation actions. This paper presents an improved total site sensitivity table (TSST) to be used as a systematic tool for this purpose. The TSST can be used to consider various 'what-if' scenarios. This tool can be used to determine the optimum size of a utility generation system, to design the backup generators and piping needed in the system and to assess the external utilities that might need to be bought and stored. The methodology is demonstrated by using an illustrated case study consisting of three processes. During the TS normal operation, the total site problem table algorithm (TS-PTA) shows that the system requires 1065 kW of high pressure steam and 645.5 kW of medium pressure steam as the heating utility, while for the cooling utility, 553.5 kW of low pressure steam and 3085 kW of cooling water are required. The results of the modified TSST proposed that a boiler and a cooling tower with the system design requiring a maximum capacity of 2.172 MW of steam and 4.1865 MW of cooling water are needed to ensure an operational flexibility between the three integrated processes.

14/02309 Decision making under uncertainty in the retrofit analysis of the UK housing stock: implications for the Green Deal

Booth, A. T. and Choudhary, R. *Energy and Buildings*, 2013, 64, 292–308.

In order to reduce carbon emissions and alleviate fuel poverty, the UK government has outlined proposals for a 'Green Deal' to help provide financing for the installation of cost-effective retrofit measures to the existing UK housing stock. However, the Green Deal proposals have the potential to generate financial risk, due to a possible overestimation of the energy savings arising from retrofit measures. This paper proposes a framework for handling the uncertainties associated with the prediction of these energy savings, as well as demonstrating how decisions can be made in the face of the uncertainties involved in the retrofit analysis of a housing stock. The proposed framework is applied to a case study set of dwellings and it is seen that a limited range of measures will be cost-effective under the Green Deal proposals for these dwellings; as a result, subsidies will be required if higher impact measures are to be considered viable. Finally, however, it is also seen that the monetary value of additional societal benefits, such as reduced carbon emissions and improved thermal comfort, is likely to more than outweigh the cost of any subsidies.

14/02310 Energy assessment of office buildings in China using LEED 2.2 and BEAM Plus 1.1

Chen, H. and Lee, W. L. *Energy and Buildings*, 2013, 63, 129–137.

LEED and BEAM Plus have been formally launched for more than 10 years. They are the two most recognized building environmental assessment schemes in China. Previous works have been done on benchmarking the energy assessment of the two schemes. However, benchmarking was either based on their earlier versions of which substantial changes have been made, or focused on their assessment issues and metrics without making reference to actual building characteristics. This paper compares the energy performance assessment results of three new office buildings in China (one in Beijing and two in Shanghai) using current versions of LEED and BEAM Plus. The three office buildings were chosen for their similarities in design. The study revealed that despite the variations in different aspects between LEED and BEAM Plus, assessment results of the three studied buildings were comparable. Amongst various building end uses, energy use for air-conditioning was found dominating the assessment results. Comparison results also show that although different tariff systems are adopted in Beijing and Shanghai, the difference will not affect the assessment results as long as same tariff system is used for predicting the energy cost of the baseline and design cases.

14/02311 Energy consumption and output: evidence from a panel of 14 oil-exporting countries

Mohammadi, H. and Parvaresh, S. *Energy Economics*, 2014, 41, 41–46.

This study examines the long-run relation and short-run dynamics between energy consumption and output in a panel of 14 oil-exporting countries over between 1980 and 2007. Panel unit root tests, which account for common cross-sectional factors, fail to reject non-stationarity in both variables. The authors explore this long-run relation and short-run dynamics using three alternative panel estimation techniques: dynamic fixed effect, pooled and mean-group estimators before and after accounting for common cross-sectional factors. These estimators allow for various degrees of heterogeneity in

long-run parameters and short-run dynamics. The results based on the mean group estimator with common correlated effects suggest: (a) a stable relation between energy consumption and output; (b) bi-directional causality in both long- and short-run; and (c) the robustness of the long-run causality results to the inclusion of additional variables. As such, environmental policies designed to curtail energy may have significant long-run ramifications for economic growth, and policies designed to promote economic growth may have adverse environmental consequences.

14/02312 Energy management strategies for multi source systems

Neffati, A. *et al. Electric Power Systems Research*, 2013, 102, 42–49.

Solving pollution problems is one of the century's challenges. Hybrid electric vehicles (HEVs) are expected to reduce significantly pollutants and consumption of fossil energy. This paper focuses on the energy management of the electric power of such HEVs. The overall objective is not only satisfying the power demand for a requested mission with several energy sources but also reducing as much as possible the hydrogen consumption with optimal splitting between the various sources, and respecting the constraints of each energy and power elements. The biggest challenge of all works that focus on energy management is to develop laws working in real time. This work presents two new energy management methods. First, an offline method called improved constraints in dynamic programming, allowing better performance than dynamic programming in terms of time computation and consumption cost is presented. Second, a real-time energy management algorithm based on fuzzy rules controller and fuzzy switching of fuzzy rules in real time will be studied. This method takes into account the evolution of the state of charge of the storage element at any time and the results obtained show, if this strategy is applied on various profiles, the consumption is near-optimal.

14/02313 Energy policymaking in Denmark: implications for global energy security and sustainability

Sovacool, B. K. *Energy Policy*, 2013, 61, 829–839.

Denmark is arguably the most energy secure and sustainable country in the Organization of Economic Cooperation and Development (OECD). The country has reduced its dependence on foreign sources of energy to zero and become self-sufficient in its own energy production and use, offering important lessons for other nations around the world. This study explores the core of Denmark's successful approach: a commitment to energy efficiency, prolonged taxes on energy fuels, electricity, and carbon dioxide, and incentives for combined heat and power and wind turbines. Through these commitments, the study shows how Denmark transitioned from being almost 100% dependent on imported fuels such as oil and coal for their power plants in 1970 to becoming a net exporter of fuels and electricity today. The country leads the world in terms of exportation of wind energy technology, with a hold on roughly one-third of the world market for wind turbines. It was able to phase out the use of virtually all oil-fired power plants in less than 5 years and implemented a progressive moratorium on future coal-fired power plants in the 1990s. Their most recent strategy seeks to achieve 30% of total energy supply from renewable energy by 2025.

14/02314 EPAR: energy performance augmented reality models for identification of building energy performance deviations between actual measurements and simulation results

Ham, Y. and Golparvar-Fard, M. *Energy and Buildings*, 2013, 63, 15–28.

Building energy performance simulation tools such as EnergyPlus, Ecotect and eQuest are widely used to model energy performance of existing buildings and assess retrofit alternatives. Nevertheless, predictions from simulations typically deviate from actual measurements. Monitoring actual performance and measuring deviations from simulated data in three dimensions can help improve simulation accuracy through model calibrations, and in turn facilitate identification of energy performance problem. To do that, this paper presents energy performance augmented reality (EPAR) modelling that leverages collections of unordered digital and thermal imagery, in addition to computational fluid dynamics (CFD) models. First, users collect large numbers of digital and thermal imagery from the building under inspection using a single thermal camera. Through an image-based reconstruction pipeline, actual three-dimensional spatio-thermal models are automatically generated and are superimposed with expected building energy performance models generated using CFD analysis through a user-driven process. The outcomes are EPAR models which visualize actual and expected models in a common three-dimensional environment. Within the EPAR models, actual measurements and simulated results can be systematically compared and analysed. The method is validated on typical residential and instructional buildings. The results demonstrate that EPAR models facilitate calibration of building energy performance models and support detection and analysis of building performance deviations.

14/02315 Evaluating the evaluations: evidence from energy efficiency programmes in Germany and the UK

Rosenow, J. and Galvin, R. *Energy and Buildings*, 2013, 62, 450–458.

To make robust judgements of an energy efficiency programme's economic effectiveness, one needs to know how much energy and CO_2 is actually being saved through the financial support it provides. But most evaluations of home retrofit energy efficiency programmes depend on calculated, rather than measured, levels of energy consumption. This fails to take into account the discrepancies that have been observed in practice, between calculated and actual energy consumption both before and after refurbishment. Evaluations of energy efficiency programmes ideally need to consider rebound effects, free rider effects, reduced savings due to insufficient technical quality, and discrepancies between actual and calculated pre-refurbishment energy consumption. This paper investigates and compares evaluations of two prominent energy efficiency programmes in Germany and the UK: the CO_2-Building Rehabilitation Programme and the Supplier Obligation. The authors show that evaluations of the Supplier Obligation explicitly address most of the reduction effects whereas this is not the case for the CO_2-Building Rehabilitation Programme.

14/02316 Expert elicitations of energy penalties for carbon capture technologies

Jenni, K. E. *et al. International Journal of Greenhouse Gas Control*, 2013, 12, 136–145.

This paper describes the results of expert assessments about the range of likely energy penalties (EP), the energy required to capture and compress CO_2, for coal power plants in 2025 for six capture technologies under three different policy scenarios. Expert opinions about the EP of each technology varied substantially. Measuring EP in terms of the fractional decrease in output per unit input, it was found that a scenario of worldwide carbon pricing leads to a decrease in the mean energy penalty of 1–10% across the technologies, and a scenario of increased US government research and development (R&D) funding leads to a decrease in the mean energy penalty of 6–14%. EP for pre-combustion capture showed the smallest improvement from R&D and carbon pricing, while EP for post-combustion capture with membranes or 'other' approaches showed the largest improvement. Although other factors will also affect costs, EP is a large component and these results suggest that capture costs are likely to fall both through investments in research and through the process of commercializing the technology in response to carbon prices. The challenges for each technology that were described by the experts, as well as the quantitative results, are described.

14/02317 From the new European Standards to an environmental, energy and economic assessment of building assemblies from cradle-to-cradle (3E-C2C)

Silvestre, J. D. *et al. Energy and Buildings*, 2013, 64, 199–208.

This paper proposes a method to aid in the comparison and choice of alternatives for assemblies closely related to the thermal performance of buildings. The method provides an assessment of the environmental, energy and economic life cycle from cradle to cradle (3E-C2C) following recent European standards for the environmental and economic assessment of construction works. Environmental performance is assessed using life cycle assessment method, energy performance corresponds to consumption of energy for heating and cooling, and the economic performance is based on the whole-life costing (WLC) method. The 3E cost-C2C approach establishes weights that allow the quantification of each aspect of the assembly's performance using the same unit. This approach uses a prevention-based environmental impact assessment method that converts the results of all impact categories into an economic unit. This allows the cost of the environmental impacts to be added to the economic and energy WLC and a 3E performance C2C to be considered, therefore preventing contradictory conclusions that can arise from the individual analysis of each aspect. 3E-C2C is useful in the selection of an external wall alternative, and corresponding insulation thickness, when comparing alternatives that are not functionally equivalent, since there is no need to change their characteristics to make them comparable.

14/02318 Global wind power development: economics and policies

Timilsina, G. R. *et al. Energy Policy*, 2013, 61, 642–652.

The existing literature indicates that theoretically, the Earth's wind energy supply potential significantly exceeds global energy demand. Yet, only 2–3% of global electricity demand is currently derived from wind power despite 27% annual growth in wind-generating capacity over the past 17 years. More than 95% of total current wind power capacity is installed in developed countries, China and India. The analysis shows that the economic competitiveness of wind power varies

at a wider range across countries or locations. A climate change damage cost of US$20/tCO$_2$ imposed on fossil fuels would make onshore wind competitive to all fossil fuels for power generation; however, the same would not happen to offshore wind, with few exceptions, even if the damage cost is increased to US$100/tCO$_2$. To overcome a large number of technical, financial, institutional, market and other barriers to wind power, many countries have employed various policy instruments, including capital subsidies, tax incentives, tradable energy certificates, feed-in tariffs, grid access guarantees and mandatory standards. Climate change mitigation policies, such as the clean development mechanism, have played a pivotal role in promoting wind power. Despite these policies, intermittency, the main technical constraint, could remain as the major challenge to the future growth of wind power.

14/02319 Highly-resolved modeling of personal transportation energy consumption in the United States

Muratori, M. *et al. Energy*, 2013, 58, 168–177.

This paper focuses on the estimation of the total primary energy consumption for personal transportation in the USA, to include gasoline and/or electricity consumption, depending on vehicle type. The bottom-up sector-based estimation method introduced here contributes to a computational tool under development at Ohio State University for assisting decision making in energy policy, pricing and investment. In order to simulate highly resolved consumption profiles, three main modelling steps are needed: modelling the behaviour of drivers, generating realistic driving profiles and simulating energy consumption of different kinds of vehicles. The modelling proposed allows for evaluating the impact of plug-in electric vehicles on the electric grid – especially at the distribution level. It can serve as a tool to compare different vehicle types and assist policy-makers in estimating their impact on primary energy consumption and the role transportation can play to reduce oil dependency.

14/02320 How do the stock prices of new energy and fossil fuel companies correlate? Evidence from China

Wen, X. *et al. Energy Economics*, 2014, 41, 63–75.

This study documents the return and volatility spillover effect between the stock prices of Chinese new energy and fossil fuel companies using the asymmetric BEKK model. Based on daily samples taken from 30 August 2006 to 11 September 2012, the dynamics of new energy/fossil fuel stock spillover are found to be significant and asymmetric. Compared with positive news, negative news about new energy and fossil fuel stock returns leads to larger return changes in their counter assets. News about both new energy and fossil fuel stock returns spills over into variances of their counter assets, and the volatility spillovers depend complexly on the respective signs of the return shocks of each asset. The empirical results demonstrate that new energy and fossil fuel stocks are generally viewed as competing assets, that positive news about new energy stocks could affect the attractiveness of fossil fuel stocks and that new energy stock investment is more speculative and riskier than fossil fuel stock investment. These results have potential implications for asset allocation, financial risk management and energy policymaking.

14/02321 Modeling of the energy demand of the residential sector in the United States using regression models and artificial neural networks

Kialashaki, A. and Reisel, J. R. *Applied Energy*, 2013, 108, 271–280.

This paper describes the development of energy-demand models which are able to predict the future energy demand in the residential sector of the USA. One set of models use an artificial neural network technique, and the other set of models use a multiple linear regression technique. The models are used to forecast future household energy demand considering different scenarios for the growth rates of the effective factors in the models. The household sector includes all energy-consuming activities in residential units (both apartments and houses) including space and water heating, cooling, lighting and the use of appliances. In order to understand the evolution of household energy use, a set of indicators has been developed. For instance, several factors affect energy consumption for space heating as a share of households' energy demand. These factors include, dwelling size, number of occupants, the efficiency of heating equipment and the useful energy intensity. The paper also analyses the trend of energy consumption in the residential sector of the USA. Moreover, the effects of important indicators on the energy consumption are discussed. The analysis performed in this paper is done for each census region, where possible, to elucidate the effects of different indicators in each region.

14/02322 Reference criteria for the identification of accident scenarios in the framework of land use planning

Tugnoli, A. *et al. Journal of Loss Prevention in the Process Industries*, 2013, 26, (4), 614–627.

Land-use planning (LUP) around industrial sites at risk of major accidents requires the application of sound approaches in the selection of credible accident scenarios. In fact, the 'technical' phase of LUP is based on the identification and assessment of relevant accident scenarios. An improper choice of scenarios may critically affect both the 'technical' phase of risk assessment and the following 'policy' phase concerning decision making on land-use restrictions and/or licensing. The present study introduces a procedure aimed at the systematic identification of reference accident scenarios to be used in the gathering of technical data on potential major accidents, which is a necessary step for LUP around Seveso sites. Possible accident scenarios are generated by an improved version of the Methodology for the Identification of Major Accident Hazards methodology. The accident scenarios are then assessed for LUP relevance considering severity, frequency and time-scale criteria. The influence of prevention and mitigation barriers is also taken into account. Two applications are used to demonstrate the proposed procedure. In both case studies, the proposed methodology proved successful in producing consistent sets of reference scenarios.

14/02323 Technology variation vs. R&D uncertainty: what matters most for energy patent success?

Popp, D. *et al. Resource and Energy Economics*, 2013, 35, (4), 505–533.

Research and development (R&D) is an uncertain activity with highly skewed outcomes. Nonetheless, most recent empirical studies and modelling estimates of the potential of technological change focus on the average returns to R&D for a composite technology and contain little or no information about the distribution of returns to R&D – which could be important for capturing the range of costs associated with climate change mitigation policies – by individual technologies. Through an empirical study of patent citation data, this paper adds to the literature on the outcomes of energy R&D by focusing on the behaviour of the most successful innovations for six energy technologies, allowing us to determine whether uncertainty or differences in technologies matter most for success. Two key results are highlighted. First, the authors compared the results from an aggregate analysis of six energy technologies to technology-by-technology results. The results show that existing work that assumes diminishing returns but assumes one generic technology is too simplistic and misses important differences between more successful and less successful technologies. Second, quantile regression techniques were used to learn more about patents that have a high positive error term in the regressions – that is, patents that receive many more citations than predicted based on observable characteristics. The authors found that differences across technologies, rather than differences across quantiles within technologies, are more important. The value of successful technologies persists longer than those of less successful technologies, providing evidence that success is the culmination of several advances building upon one another, rather than resulting from one single breakthrough. Diminishing returns to research activities appear most problematic during rapid increases of research investment, such as experienced by solar energy in the 1970s.

14/02324 The Fukushima nuclear accident and its effect on global energy security

Hayashi, M. and Hughes, L. *Energy Policy*, 2013, 59, 102–111.

The March 2011 nuclear accident at the Fukushima Daiichi nuclear power station affected both short- and long-term energy-security in Japan, resulting in crisis-driven, *ad hoc* energy policy and, because of the decision to shutter all nuclear reactors, increased the country's demand for fossil fuels, primarily natural gas. However, the effects of the accident on energy security were not restricted to Japan; for example, the worldwide availability and affordability of liquefied natural gas were affected by Japan's increased demand; while the accident itself resulted in the loss of public acceptability of nuclear power and led countries, such as Germany and Italy, to immediately shut down some of the nuclear reactors or abandon plans to build new ones. This paper examines some of the short-term effects on global energy security following the accident at Fukushima, focusing on the main replacement fuel, liquefied natural gas. It shows, among other things, that the accident increased investment in liquefied natural gas projects around the world. The paper shows that despite Fukushima contributing to nuclear power's loss of acceptability in most developed countries, it is still seen as an essential way of improving energy security in many countries and, despite what its critics may say, will probably continue to be used as a significant source of low-carbon electricity.

14/02325 The interdependence of European–Russian energy relations

Harsem, Ø. and Claes, D. H. *Energy Policy*, 2013, 59, 784–791.

The aim of this article is to explore this dynamic interdependent relationship between Russia and Europe in the field of energy. Based on the concept of interdependence and perspectives on the political aspects of trade relations the authors discuss how Russia can exercise

power based on its energy resources and how the European Union (EU) can compensate for its lack of power in the energy game with other trade related capabilities. In particular they explore the implications of the lack of a full-fledged EU foreign energy policy towards Russia, with the somewhat counter-intuitive conclusion that the EU countries, on average, not necessarily are better off with a common foreign energy policy.

14/02326 Volatility forecasting and risk management for commodity markets in the presence of asymmetry and long memory
Chkili, W. *et al. Energy Economics*, 2014, 41, 1–18.
This paper explores the relevance of asymmetry and long memory in modelling and forecasting the conditional volatility and market risk of four widely traded commodities (crude oil, natural gas, gold and silver). A broad set of the most popular linear and non-linear GARCH-type models is used to investigate this relevancy. The in-sample and out-of-sample results show that volatility of commodity returns can be better described by non-linear volatility models accommodating the long memory and asymmetry features. In particular, the FIAPARCH model is found to be the best suited for estimating the value at risk forecasts for both short and long trading positions. This model also gives for all four commodities the lowest number of violations under the Basel II Accord rule, given a risk exposure at the 99% confidence level. Several implications for commodity market risks, policy regulations and hedging strategies can be drawn from the obtained results.

Energy conservation

14/02327 A study of the rebound effect on China's current energy conservation and emissions reduction: measures and policy choices
Lin, B. *et al. Energy*, 2013, 58, 330–339.
Energy efficiency improvement leads to a reduction in the real cost of energy services per unit, thus bringing about an increase in the demand for energy services. Therefore, the potential energy savings and emission reduction from efficiency improvements might be offset, which is known as the 'rebound effect'. This study disaggregates the effect into the direct and indirect effects based on the Slutsky equation and finds that the rebound effect of Chinese urban households is approximately 22%. It is found that the indirect effect is stronger than the direct effect. These findings prove that the initial goals of the government on energy conservation and emission reduction could not be achieved by improving energy efficiency alone, but need to be supplemented with relevant energy pricing reforms.

14/02328 An Italian input–output model for the assessment of energy and environmental benefits arising from retrofit actions of buildings
Cellura, M. *et al. Energy and Buildings*, 2013, 62, 97–106.
The paper presents an energy and environmental extended input–output model combined with a life cycle assessment, applied to assess the energy and environmental benefits arising from the Italian policy of tax deduction for energy retrofits of buildings. The study allowed the assessment of the advantages of the above policy, taking into account both direct and indirect energy saving and avoided CO_2 emissions obtained with the retrofit actions and indirect energy consumption and related CO_2 emissions due to the realization of the above actions. Moreover, the authors defined an original model to assess the indirect rebound effect caused by the energy saving actions. The obtained results showed that a reliable evaluation of the benefits arising from sustainable policies strongly depends on the indirect rate of the energy consumption and energy saving, that in the examined case study has the same order of magnitude of the direct one, and on the rebound effect, that can partially avoid the obtained benefits. The study represents one of the first Italian experiences aimed at assessing the effectiveness of sustainable production and consumption strategies. It can be used to support decision-makers in the selection of policies aimed at reducing energy and environmental impacts caused by final consumptions.

14/02329 Analysis of energy saving potential of air-side free cooling for data centers in worldwide climate zones
Lee, K.-P. and Chen, H.-L. *Energy and Buildings*, 2013, 64, 103–112.
Based on the climate classification of ASHRAE 90.1 and the required operating environment conditions for data centres suggested by the ASHRAE Technical Committee TC 9.9, a dynamic building energy simulation program was used to examine the potential energy savings of the air-side free cooling technology with differential enthalpy control used in data centres in 17 climate zones. The results showed that significant free cooling potential was achieved in data centres located in mixed-humid, warm-marine, and mixed-marine climate zones. Because significant humidification is required to adjust outdoor air in climate zones with a lower dew point temperature, such as very-cold, subarctic, cool-dry, and cold-dry climate zones, the power consumed is even higher. Although the cooling degree day (CDD) and heating degree day (HDD) are key factors of climate classification and air conditioning energy consumption, they are not entirely correlated to the specific operating environment conditions of data centres. The results of this study showed that for every 2 °C decline in the indoor temperature of a data centre, the energy saving of free cooling technology may decrease by 2.8–8.5%. The rate of decline varies in different climate zones.

14/02330 Applying data envelopment analysis approach to improve energy efficiency and reduce GHG (greenhouse gas) emission of wheat production
Khoshnevisan, B. *et al. Energy*, 2013, 58, 588–593.
In this study, data envelopment analysis was applied to analyse the energy efficiency of wheat farms in order to separate efficient and inefficient growers and to calculate the wasteful uses of energy. Additionally, the degrees of technical efficiency, pure technical efficiency and scale efficiency were determined. Furthermore, the effect of energy optimization on greenhouse gas (GHG) emissions was investigated and the total amount of GHG emissions of efficient farms was compared with inefficient ones. Based on the results it was revealed that 18% of producers were technically efficient and the average of technical efficiency was calculated as 0.82. Based on the Banker–Charnes–Cooper model, 154 growers (59%) were identified efficient and the mean pure technical efficiency of these farmers was found to be 0.99. Also, it was concluded that 2075.8 MJ ha^{-1} of energy inputs can be saved if the performance of inefficient farms rises to a high level. Additionally, it was observed that the total GHG emission from efficient and inefficient producers was 2713.3 and 2740.8 kg $CO_{2eq.}\,ha^{-1}$, respectively. By energy optimization the total GHG emissions can be reduced to the value of 2684.29 kg $CO_{2eq.}\,ha^{-1}$.

14/02331 Bus HVAC energy consumption test method based on HVAC unit behavior
Hegar, M. *et al. International Journal of Refrigeration*, 2013, 36, (4), 1254–1262.
This paper presents a test method for determination of energy consumption of a bus's heating, ventilation and air-conditioning (HVAC) unit. The energy consumption corresponds to a bus engine fuel consumption increase during the HVAC unit operation period. The HVAC unit energy consumption is determined from the unit input power, which is measured under several levels of bus engine speeds and at different levels of testing heat load in the laboratory environment. Since the bus engine fuel consumption is incrementally induced by powering an HVAC unit, the results are subsequently recalculated to the unit fuel consumption under the defined road cycles in terms of a standardized diesel engine. The method is likewise applicable either for classic or electric HVAC units with a main consumer (compressor or high-voltage alternator) mechanically driven directly from the bus engine and also for electric HVAC units supplied from an alternative electric energy source in case of hybrid or fully electric buses.

14/02332 Comparative assessment of internal and external thermal insulation systems for energy efficient retrofitting of residential buildings
Kolaitis, D. I. *et al. Energy and Buildings*, 2013, 64, 123–131.
A comparative assessment of internal versus external thermal insulation systems for energy efficient retrofitting of residential buildings is performed by means of detailed numerical simulations. A 99.6 m^2 one-storey apartment located at a mid-level of a multi-storey building is utilized as a 'benchmark' case; the external walls of the building are considered to be non-insulated, a typical condition for the majority of the existing Greek building stock, which has been constructed before 1980. The annual thermal and cooling energy requirements are estimated by performing simulations using the TRNSYS software; the effect of insulation layer location (external, internal), meteorological conditions (warm Mediterranean and temperate Oceanic climate regions) and 'energy conscious' occupant behaviour (passive, active) is examined by means of a parametric study. Both external and internal thermal insulation configurations are found to significantly reduce the total energy requirements; on average, external insulation outperforms the internal insulation configuration by 8%. Meso-scale hygro-thermal simulations are also performed using the in-house developed HETRAN code. A significant risk for water vapour condensation emerges only in the case of internal insulation installed in the temperate Oceanic climate region. Internal insulation requires approximately 50% less investment cost than the external insulation, thus resulting in a lower payback period.

14/02333 Data association mining for identifying lighting energy waste patterns in educational institutes
Cabrera, D. F. M. and Zareipour, H. *Energy and Buildings*, 2013, 62, 210–216.
A significant portion of the energy consumption in post-secondary educational institutes is for lighting classrooms. The occupancy patterns in post-secondary educational institutes are not stable and predictable, and thus, alternative solutions may be required to match energy consumption and occupancy in order to increase energy efficiency. This paper reports an experimental research on quantifying and understanding lighting energy waste patterns in a post-secondary educational institute. Data have been collected over a full academic year in three typical classrooms. Data association mining, a powerful data mining tool, is applied to the data in order to extract association rules and explore lighting waste patterns. The simulation results show that if the waste patterns are avoided, significant savings, as high as 70% of the current energy use, are achievable.

14/02334 Design of a multipurpose 'zero energy consumption' building according to European Directive 2010/31/EU: architectural and technical plants solutions
Desideri, U. *et al. Energy*, 2013, 58, 157–167.
It is particularly important to implement policies aimed at improving energy efficiency in buildings when considering the significant impact that the residential sector has on energy consumption. Highly energy efficient buildings can either save primary energy or disseminate the use of the most suitable technologies to be used in new constructions. Due to those reasons, the municipality of Città della Pieve in Italy promoted the creation of a 'Renewable Energy Park' in a deprived area of its territory, where some green technologies could be installed and tested. This site has also been considered as an optimal location for an educational/demonstrative 'zero-energy consumption' building for multifunctional activities and realized with the most innovative techniques to save energy. The building may be considered as an example to study and optimize the benefits of higher energy efficiency together with the use of renewable energy systems. In this paper the technical solutions adopted both in the building envelope and the technical plants are described and discussed. A simulation of the behaviour of the building in summer and winter was carried out in order to assess the benefits that can be obtained both in energetic and economic terms.

14/02335 Energy conservation for international dry bulk carriers via vessel speed reduction
Chang, C.-C. and Chang, C.-H. *Energy Policy*, 2013, 59, 710–715.
This study uses an activity-based method to investigate the fuel consumption and corresponding CO_2 emissions of Capesize, Panamax, Supramax, and Handysize dry bulk carriers. The emission and energy reductions are estimated for speed reductions of 10%, 20% and 30%. The 'cost of averting a tonne of CO_2–eq heating' (CATCH) model is applied to evaluate the cost efficiency of speed reduction. Results show that speed reductions of 10%, 20% and 30% reduce fuel consumption by 27.1%, 48.8% and 60.3%, and CO_2 emissions by 19%, 36% and 51%, respectively. Speed reduction leads to emission reductions, with greater reductions for larger ships. CATCH values are positive, indicating that reducing speed increases cost. Line C3 of Capesize is used to determine the optimal ship number and operational speed under energy conservation. The minimum number of vessels in service is nine, with an average operational speed of 14.53 knots and one port call per week. If speed is reduced by 10%, 20% and 30%, one, two and four additional ships are needed, respectively.

14/02336 Estimates of electricity saving potential in Chinese nonferrous metals industry
Lin, B. and Zhang, G. *Energy Policy*, 2013, 60, 558–568.
This paper analyses the electricity saving potential of non-ferrous metals industry in China. The cointegration method is applied to estimate electricity intensity of Chinese non-ferrous metals industry, in an effort to predict future electricity saving potential. The results show that there is a long-run equilibrium between electricity intensity and factors such as R&D intensity, industrial electricity price, enterprise scale and labour productivity. By means of scenario analysis, the authors evaluate different possible measures that might be adopted to narrow down the electricity efficiency gap between non-ferrous metals industry in China and that of Japan. The results indicate that more active electricity conservation policies are needed in order to reduce the electricity intensity of Chinese non-ferrous metals industry. The authors also find that the electricity efficiency gap could be significantly narrowed by 2020 if proper electricity conservation policy is adopted. Finally, based on the results of the scenario analysis, future policy priorities are suggested.

14/02337 Estimating the energy saving potential of telecom operators in China
Yang, T.-J. *et al. Energy Policy*, 2013, 61, 448–459.
A set of models are employed to estimate the potential of total energy saved of productions and segmented energy saving for telecom operators in China. During the estimation, the total energy saving is divided into that by technology and management, which are derived from technical reform and progress, and management control measures and even marketing respectively, and the estimating methodologies for energy saving potential of each segment are elaborated. Empirical results from China Mobile indicate that, first, the technical advance in communications technology accounts for the largest proportion (70–80%) of the total energy saved of productions in telecom sector of China. Second, technical reform brings about 20–30% of the total energy saving. Third, the proportions of energy saving brought by marketing and control measures appear relatively smaller, just less than 3%. Therefore, China's telecom operators should seize the opportunity of the revolution of communications network techniques in recent years to create an advanced network with lower energy consumption.

14/02338 Information strategies and energy conservation behavior: a meta-analysis of experimental studies from 1975 to 2012
Delmas, M. A. *et al. Energy Policy*, 2013, 61, 729–739.
Strategies that provide information about the environmental impact of activities are increasingly seen as effective to encourage conservation behaviour. This paper offers the most comprehensive meta-analysis of information-based energy conservation experiments conducted to date. Based on evidence from 156 published field trials and 525,479 study subjects from 1975 to 2012, the authors quantify the energy savings from information-based strategies. On average, individuals in the experiments reduced their electricity consumption by 7.4%. The results also show that strategies providing individualized audits and consulting are comparatively more effective for conservation behaviour than strategies that provide historical, peer comparison energy feedback. Interestingly, it was found that pecuniary feedback and incentives lead to a relative increase in energy usage rather than induce conservation. It was also found that the conservation effect diminishes with the rigour of the study, indicating potential methodological issues in the current literature.

14/02339 Investigating the impact eco-feedback information representation has on building occupant energy consumption behavior and savings
Jain, R. K. *et al. Energy and Buildings*, 2013, 64, 408–414.
In response to rising energy costs and concerns over environmental emissions, researchers and practitioners have developed eco-feedback systems to provide building occupants with information on their energy consumption. While such eco-feedback systems have been observed to drive significant reductions in energy consumption, little is known as to what specific design features of these systems are most motivational. One common feature of eco-feedback systems is the way in which energy consumption is represented to users. This study empirically examines the impact that information representation has on energy consumption behaviour by comparing the effectiveness of direct energy feedback versus feedback represented as an environmental externality. A one-month empirical study with 39 participants in an urban residential building was conducted. Participants were divided into two different study groups: one group was provided with feedback in direct energy units and a second group was provided feedback in environmental externality units. Results revealed that information representation has a statistically significant impact on the energy consumption behaviour of users, and that users receiving eco-feedback as an environmental externality reduced their consumption more than their counterparts who received feedback in direct energy units. This study represents a crucial first step toward gaining a deeper understanding of how information representation can be leveraged to maximize energy savings.

14/02340 LCE analysis of buildings – taking the step towards net zero energy buildings
Berggren, B. *et al. Energy and Buildings*, 2013, 62, 381–391.
The basic concept of a net zero-energy building (net ZEB) is that on-site renewable energy generation covers the annual energy load. The main objective of this study is to analyse the increase of embodied energy compared to the decrease of the energy use related to building operation; partly by a literature review, partly by detailed analysis of 11 case studies; taking the step from a low energy building to a net ZEB. The literature review shows that the metric of evaluation, assumed life-span, boundary conditions, age of database and the origin of database differ in different studies and influence the result of embodied energy. The relationship between embodied energy and life cycle energy use is almost linear for all cases studied herein. During the last two decades, embodied energy in new buildings has decreased slightly. However, the relative share of embodied energy related to life cycle energy use has increased. The detailed life cycle energy analysis show that taking the step from a low energy building to a net ZEB results in a small increase

of the embodied energy. However, the energy savings achieved in the annual operating energy balance clearly exceed the increase in embodied energy.

14/02341 Monitoring the performance of low energy dwellings: two UK case studies

Guerra-Santin, O. *et al. Energy and Buildings*, 2013, 64, 32–40.

Recent studies show a mismatch between expected and actual performance in low energy buildings. The differences have been attributed to occupant behaviour and poor quality of the construction. Monitoring building performance during and after construction can ensure that systems and fabric perform as designed. This study sought to evaluate the delivery process of low energy dwellings including the energy and environmental monitoring processes and the performance of the building itself. The study focused on the post-construction phase of the building process and consists of a construction review, as well as fabric and system performance tests. The results of the tests show that the dwellings perform close to design expectations. However, the performance monitoring highlighted issues that could have undermined their performance. The results of the study stress the utility of monitoring activities in low energy buildings, and specifically the need for monitoring low carbon technologies. Recommendations are given to improve the efficiency of monitoring processes in low energy dwellings.

14/02342 Role of PCM based nanofluids for energy efficient cool thermal storage system

Kumaresan, V. *et al. International Journal of Refrigeration*, 2013, 36, (6), 1641–1647.

This study presents the solidification behaviour of a water-based nanofluid-phase change material (NFPCM) encapsulated in a spherical container. The NFPCM was prepared by dispersing the multi-wall carbon nanotubes (MWCNT) with volume fractions of 0.15%, 0.3%, 0.45% and 0.6% in deionized (DI) water as the base phase change material (PCM). The solidification experiments were conducted with DI water and the NFPCM and maximum reductions of 14% and 20.1% were observed in the solidification time with the NFPCMs at surrounding bath temperature of −9 and −12 °C, respectively. The presence of MWCNT also acted as nucleating agent that caused appreciable reduction in the subcooling. The enhanced thermal transport properties of the NFPCM are very useful to operate the cool thermal energy storage (CTES) system at higher operating temperature of the secondary refrigerant. It is predicted that there is a possible energy saving potential of approximately 6–9% in the CTES using the NFPCMs.

17 ENERGY CONVERSION AND RECYCLING

14/02343 A study of the pyrolysis behaviors of pelletized recovered municipal solid waste fuels

Zhou, C. *et al. Applied Energy*, 2013, 107, 173–182.

Pelletized recovered solid waste fuel is often applied in gasification systems to provide feedstock with a stabilized quality and high heating value and to avoid the bridging behaviour caused by high moisture content, low particle density, and irregular particle size. However, the swelling properties and the sticky material generated from pyrolysis of the plastic group components also tend to trigger bridging in the retorting zone. It is well known that the plastic group materials, which occupy a considerable proportion of municipal solid waste, can melt together easily even under low temperature. This study investigates the pyrolysis behaviours of typical recovered solid waste pellets, including the devolatilization rate, heat transfer properties, char properties, and swelling/shrinkage properties, in a small fixed-bed facility over a wide temperature range, from 900 to 450 °C. The results are also compared with those from wheat straw pellets, a typical cellulosic fuel. Moreover, the SEM images and BET analysis of the char structure are further analysed to provide additional explanation for the mechanisms of swelling/shrinkage phenomena observed during heating.

14/02344 Agricultural residue production and potentials for energy and materials services

Bentsen, N. S. *et al. Progress in Energy and Combustion Science*, 2014, 40, 59–73.

Agricultural residues are potentially major contributors of resources for energy and material production. This study provides regional and global estimates of the amount of residues from major crops and addresses the sources of uncertainty in the estimation of the amount of agricultural residues produced globally. Data and methods available currently limit the use of resource estimates for energy or production planning. The authors develop function-based multipliers to estimate the global production of agricultural residues. The multipliers are applied to the production of the, on a global scale, six most important crops: barley, maize, rice, soybean, sugar cane and wheat in 227 countries and territories of the world. A global production of residues from these six crops was found to be $3.7^{+1.3}_{-1.0}$ Pg dry matter yr^{-1}. North and South America, eastern, south-eastern and southern Asia and eastern Europe each produce more than 200 Tg yr^{-1}. The theoretical energy potential from the selected crop residues was estimated to 65 EJ yr^{-1} corresponding to 15% of the global primary energy consumption or 66% of the world's energy consumption for transport. Development towards high input agriculture can increase the global residue production by ∼1.3 Pg dry matter yr^{-1}.

14/02345 Assessment of energy generation potentials of MSW in Delhi under different technological options

Chakraborty, M. *et al. Energy Conversion and Management*, 2013, 75, 249–255.

Municipal solid waste (MSW) is an important source of methane emission. Methane is a greenhouse gas and has high potential for its use as energy source. A study has been carried out to find out the energy generation potential of MSW being dumped in Delhi's three landfills, namely Ghazipur, Bhalswa and Okhla. Five technologies for waste to energy generation, namely biomethanation, incineration, gasification/pyrolysis, refused-derived fuel (RDF) and plasma arc gasification have been evaluated for computation of possible energy (WTE) generation potential of MSW under ideal conditions using the MSW specific characteristic parameters. Bulk waste with and without pre-segregation of reusable high carbonaceous materials have been considered to develop range of energy generation potentials under two scenarios of with and without segregation of MSW. USEPA-LandGem model version 3.02 has been used to get landfill gas generation potential of Delhi's landfills. The potential of biomethanation process for producing energy has been found to be in the range of 3–10, 3–8 and 2–8 MW/day from the MSW deposited in Ghazipur, Bhalswa and Okhla, respectively. The energy generation potentials of the MSW deposited in Ghazipur, Bhalswa and Okhla have been found to be in the range of 8–24, 7–22 and 7–19 MW/day for incineration process; 17–32, 16–29 and 11–25 MW/day from gasification/pyrolysis process; 9–19, 8–18 and 6–15 MW/day for RDF process; and 17–35, 16–32 and 11–28 MW/day for the plasma arc gasification process, respectively. The lower values in these ranges depict the energy generation potential for segregated waste while the higher values are for the bulk waste. These values are based on theoretical ideals and help in identifying the optimal WTE technique.

14/02346 Co-digestion of used oils and urban landfill leachates with sewage sludge and the effect on the biogas production

Pastor, L. *et al. Applied Energy*, 2013, 107, 438–445.

This paper evaluates the potential of mesophilic anaerobic digestion (AD) in the treatment of used oils and landfill leachates through co-digestion of the sludge produced in a wastewater treatment plant (WWTP). Biomethane potential (BMP) tests were performed on two different co-substrates and on WWTP sludge. The biogas production per kg of fresh matter of the sludge generated in a WWTP was only 6.1 Nl/kg due to its low volatile solids concentration. Biogas production of landfill leachates per kg of fresh matter was found to be low (12.4 Nl/kg). The biogas production per kg of fresh matter for the used oil over a period of 47 days (not completely degraded) was 970.6 Nl/kg. Used oil was selected as co-substrate according to these results. Anaerobic co-digestion of sludge and used oil was conducted in a pilot plant fed in semi-continuous regime in the mesophilic range (38 °C) to obtain their adequate mixture in order to ensure the correct function of the process. The optimum oil percentage in the mixture was 19% (volatile solids basis). Once the appropriate mixture was obtained the co-digestion process was carried out in the digester of the Pobla de Farnals WWTP. The co-digestion process improved the performance of volatile matter removal (showing an 11% increase over the period without co-digestion) as well as the biogas production (a 23.5% increase over the period without co-digestion) without disturbing the anaerobic digestion process. The total production of biogas per day in the WWTP increased over the period without co-digestion.

14/02347 Energy and exergy analyses of a bottoming Rankine cycle for engine exhaust heat recovery

Zhu, S. *et al. Energy*, 2013, 58, 448–457.

In this paper, a theoretical study on the thermodynamic processes of a bottoming Rankine cycle for engine waste heat recovery is conducted from the viewpoints of energy balance and exergy balance. A theoretical formula and an exergy distribution map for qualitative analyses of the main operating parameters are presented under simplified conditions when exhaust gas is selected as the only heat source. Five typical working fluids, which are always selected by

manufacturers for different types of engines, are compared under various operating conditions in Matlab software. The results show that working fluid properties, evaporating pressure and superheating temperature are the main factors influencing the system design and performances. The global recovery efficiency does not exceed 0.14 under typical operating conditions. Ethanol and R113 show better thermodynamic performances in the whole exhaust gas temperature range. In addition, the optimal evaporating pressure usually does not exist in engine exhaust heat recovery, and the distributions of exergy destruction are varied with working fluid categories and system design constraints.

14/02348 From waste to energy: microalgae production in wastewater and glycerol

Cabanelas, I. T. D. *et al. Applied Energy*, 2013, 109, 283–290.

This study evaluates the auto/mixotrophic growth of microalgae using domestic wastewater amended with glycerol aiming biofuels production. The best results were obtained with the highest glycerol supplementation (50 mM). In such condition, *Chlorella vulgaris* and *Botryococcus terribilis* showed a biomass productivity of 118 and 282 $mg\,l^{-1}\,d^{-1}$, which produced about 18 and 35 $mg\,l^{-1}\,d^{-1}$ of lipids, respectively. Thus, if scaled-up (200 $m^3\,d^{-1}$ of WW, 240 working days y^{-1}) biomass and lipid yields may be about 5.6 $tons\,y^{-1}$ and 894.2 $kg\,y^{-1}$ or 13.5 $tons\,y^{-1}$ and 1.6 $tons\,y^{-1}$ for *C. vulgaris* and *B. terribilis*, respectively. The mixotrophic production of lipids can generate high quality biodiesel according to estimations using their fatty acids profiles. The whole process can be advantageously combined with the production of other biofuels (e.g. methane and bio-ethanol) in a biorefinery scenario. This combination of algal biomass production with waste treatment (wastewater amended with glycerol) can have a significant impact in the water treatment sector and local markets.

14/02349 Investigation on a ventilation heat recovery exchanger: modeling and experimental validation in dry and partially wet conditions

Gendebien, S. *et al. Energy and Buildings*, 2013, 62, 176–189.

The present paper focuses on the development and experimental validation of a model of air-to-air heat exchanger dedicated to domestic mechanical heat recovery ventilation. The proposed model describes dry and partially wet regimes. The first part of the paper presents a semi-empirical model based on the physical characteristics of the heat recovery device and relying on empirical correlations available in the literature for the convective heat transfer coefficients. In the case of partially wet regime, a moving boundary model is applied in order to predict sensible and latent heat transfer rates. A model developed with friction factor coefficients estimated by correlations from the literature is also presented in order to predict the hydraulic performance in dry conditions. The second part of the paper describes the experimental investigation conducted on an off-the-shelf heat exchanger. Experimental data are used to tune correlations for the determination of the convective heat transfer coefficient and validate the proposed simulation model of the ventilation heat recovery exchanger in partially wet conditions. The model developed to determine the hydraulic performance with existing correlations for the friction factor coefficient does not require a calibration. Finally, examples of use of the developed model are presented, which includes coupling the model with a building simulation model, a study of the influence of the humidity on the evolution of the latent and sensible heat transfer rates and strategies to avoid freezing in the heat exchanger.

14/02350 Kinetics and mechanisms of hydrogen sulfide adsorption by biochars

Shang, G. *et al. Bioresource Technology*, 2013, 133, 495–499.

Three different biochars as cost-effective substitutes for activated carbon (AC) were tested for their hydrogen sulfide (H_2S) adsorption ability. The biochars were produced from camphor (SC), bamboo (SB), and rice hull (SR) at 400 °C by oxygen-limited pyrolysis. The surface area (SA), pH, and Fourier transform infrared spectras of the biochars and AC were compared. The maximum removal rates and the saturation constants were obtained using the Michaelis–Menten-type equation. The three biochars were found to be alkaline, and the SAs of the biochars were much smaller than that of the AC. The H_2S breakthrough capacity was related to the local pH within the pore system of the biochar. The order observed in terms of both biochar and AC adsorption capacity was SR > SB > SC > AC. SR efficiently removed H_2S within the inlet concentration range of 10–50 μL/L. Biochars derived from agricultural/forestry wastes are a promising H_2S adsorbent with distinctive properties.

14/02351 Microwave pyrolysis of polymeric materials: waste tires treatment and characterization of the value-added products

Undri, A. *et al. Journal of Analytical and Applied Pyrolysis*, 2013, 103, 149–158.

Waste tyres are well known to have relevant disposal or reprocessing problems under environmental and economic sustainable conditions. These processes may be a challenge for industrial and academic research. In this context, pyrolysis represents a modern, valid alternative treatment for waste tyres as long as it will be possible to generate value-added products. Improvements in heat-transfer technology are crucial in order to optimize the efficiency of the process itself. Here, the authors describe the use of microwave (MW) irradiation as one of the most promising heating technologies for pyrolysis, due to its ability to heat quickly and directly any MW-absorbing material. Experiments were run in a batch laboratory scale with an oven operating at a frequency of 2.45 GHz with a variable energy output up to 6 kW. A special attention was dedicated to the influence of operating variables on liquid product properties. The reaction was performed in a short time comparing with traditional heating techniques and the most performing conditions were achieved using a MW power of 3 kW per 0.2 kg of tyres. Typical products were a solid residue (char) containing up to 92.03% of carbon and appreciable quantities of mineral matter, a low viscosity oil (<2.9 cP, with a large number of single-ring aromatic hydrocarbons) and a gas containing light hydrocarbons, hydrogen and only traces of N_2. The three products collected had high calorific values: 34 MJ/kg for solid, 45 MJ/kg for liquid and 46 MJ/kg for the gas fraction, respectively.

14/02352 Multi-objective optimization of organic Rankine cycles for waste heat recovery: application in an offshore platform

Pierobon, L. *et al. Energy*, 2013, 58, 538–549.

This study examines the optimal design of a megawatt-size organic Rankine cycle by employing the multi-objective optimization with the genetic algorithm as the optimizer. The authors consider three objective functions: thermal efficiency, total volume of the system and net present value. The optimization variables are the working fluid, the turbine inlet pressure and temperature, the condensing temperature, the pinch points and the fluid velocities in the heat exchangers. The optimization process also includes the complete design of the shell and tube heat exchangers utilized in the organic Rankine cycle. The methodology is applied to recover the waste heat from the SGT-500 gas turbine installed on the Draugen offshore oil and gas platform in the North Sea. Results suggest two optimal working fluids, i.e. acetone and cyclopentane. Thermal efficiency and net present value are higher for cyclopentane than for acetone. Other promising working fluids are cyclohexane, hexane and isohexane. This methodology can be used in waste heat recovery applications where a compromise between performance, compactness and economic revenue is required.

14/02353 Production of elemental sulfur from sulfide and nitrate-laden wastewaters by methanogenic culture via sulfide denitrifying removal process

Nanda, J. *et al. Biochemical Engineering Journal*, 2013, 78, 128–131.

The denitrifying sulfide removal (DSR) process is a biorefinery process that can produce colloidal S^0 from sulfide and nitrate-laden wastewaters. At long reaction times, the formed S^0 is reduced back to sulfide by sulfate-reducing bacteria, resulting in a poor conversion rate of S^0. The presence of optimal hydraulic retention time (HRT) for maximizing S^0 conversion from DSR wastewaters was proposed by batch assays and then confirmed in continuous flow tests.

14/02354 Recuperator for waste heat recovery from rotary kilns

Karamarković, V. *et al. Applied Thermal Engineering*, 2013, 54, (2), 470–480.

The energy balance of a rotary kiln used for calcination of dolomite in a magnesium production company identified the kiln shell (26.35% of the input energy) and exhaust gases (18.95%) as the major sources of heat losses. To decrease the heat loss, a heat exchanger that forms an annular duct over the calcination zone of the kiln is used to preheat combustion air. The exchanger uses both the convective and radiant heat loss from the mantle, prevents overheating, does not require air tightness, and could be implemented over rotary kilns with the similar surface temperature distribution. A mathematical model that defines the geometry of the heat exchanger so as the heat transfer from the kiln to the combustion air to be equal to the heat dissipated from the bare kiln is presented. The exchanger decreases fuel consumption of the kiln for 12.00%, and increases its energy and exergy efficiency for 7.35% and 3.81%, respectively. To obtain a better performance the airflow and geometry of the exchanger should be arranged to achieve the smallest possible temperature difference between the kiln surface and the preheating air, whose amount should always be kept at the optimal value for the used fuel.

14/02355 Risk identification for PPP waste-to-energy incineration projects in China

Song, J. *et al. Energy Policy*, 2013, 61, 953–962.

Municipal solid waste (MSW) is regarded as a renewable energy source. In China, the sharp increase of MSW has precipitated the rapid growth of waste-to-energy (WTE) incineration plants. Private capital has been getting into the WTE incineration industry through the public–private partnership (PPP) arrangement. Due to the large construction cost and the long concession period commonly associated with this arrangement, a number of failures have emerged in PPP WTE incineration projects. The aim of this paper is to investigate the key risks of PPP WTE incineration projects in China and study the strategies for managing these risks by drawing experience and learning lessons from these projects. First, the authors analysed the MSW management practices, relevant legislations and policies, and the development of PPP WTE incineration projects in China. Second, they identified 10 key risks through interviews, surveys and visits to some selected projects, and provided detailed analysis of these risks. Lastly, the authors developed response strategies for these risks from the perspectives of both public and private sectors.

14/02356 Simulation and optimization of waste heat recovery in sinter cooling process

Zhang, X. *et al. Applied Thermal Engineering*, 2013, 54, (1), 7–15.

The particle size, the gaseous velocity and temperature at the inlet, and the porosity and the height of the sintered bed are the five main parameters affecting the efficiency of the waste heat recovery in a sinter cooling process. A numerical model was developed on the basis of the porous media model and local non-equilibrium thermodynamics model, to reveal the flow and heat transfer characteristics of a $420\,m^2$ sinter cooler in an iron and steel company with the software package Fluent 6.3. Simulation was carried out and influences of different parameters on the distribution of solid temperature, the gaseous temperature and velocity, and the waste heat utilization were discussed. The reliability of this model was verified by comparing the prediction data with the experimental data. In order to investigate the influence of multi-layer feeding on waste heat utilization, 10 parameters including the above five were optimized with the mixed orthogonal experimental method. The significance degree of the parameters was obtained. The optimal combination of the parameters was proposed in the purpose of improving the waste heat utilization. The amount of waste heat utilization is 2.5531×10^8 kJ/h in the optimal condition, which increases 26.26% compared to the standard condition.

14/02357 Supercapacitors based on carbons with tuned porosity derived from paper pulp mill sludge biowaste

Wang, H. *et al. Carbon*, 2013, 57, 317–328.

Hydrothermal carbonization followed by chemical activation is utilized to convert paper pulp mill sludge biowaste into high surface area (up to $2980\,m^2\,g^{-1}$) carbons. This synthesis process employs an otherwise unusable byproduct of paper manufacturing that is generated in thousands of tons per year. The textural properties of the carbons are tunable by the activation process, yielding controlled levels of microporosity and mesoporosity. The electrochemical results for the optimized carbon are very promising. An organic electrolyte yields a maximum capacitance of $166\,F\,g^{-1}$, and a Ragone curve with $30\,W\,h\,kg^{-1}$ at $57\,W\,kg^{-1}$ and $20\,W\,h\,kg^{-1}$ at $5450\,W\,kg^{-1}$. Two ionic liquid electrolytes result in maximum capacitances of $180–190\,F\,g^{-1}$ with up to 62% retention between 2 and $200\,mV\,s^{-1}$. The ionic liquids yielded energy density–power density combinations of $51\,W\,h\,kg^{-1}$ at $375\,W\,kg^{-1}$ and $26–31\,W\,h\,kg^{-1}$ at $6760–7000\,W\,kg^{-1}$. After 5000 plus charge–discharge cycles the capacitance retention is as high at 91%. The scan rate dependence of the surface area normalized capacitance highlights the rich interplay of the electrolyte ions with pores of various sizes.

14/02358 Sustainability issues of plutonium recycling in light water reactors: code evaluations up to 2050

Calabrese, R. *Annals of Nuclear Energy*, 2013, 58, 268–271.

Plutonium recycling in light water reactors is a viable and mature technology capable of improving several indicators of great importance in the evaluation of the sustainability of nuclear energy development in the near- and long-term such as the shortage of natural uranium resources, the increase of spent fuel inventories and the proliferation risks of high-level radioactive waste. This paper, after a brief review of the status of plutonium recycling, presents the results of a scenario analysis carried out in the hypothesis that the share of nuclear fleet loaded with mixed uranium–plutonium oxide fuel (MOX) is kept constant up to the middle of the century. Beside mentioned indicators, the paper discusses the needs for complex and costly fuel cycle infrastructures required for the reprocessing of spent nuclear fuel and the fabrication of MOX. Assuming that the deployment of fast reactors occurs beyond the middle of the century, the article focuses on the comparison of an open fuel cycle strategy with a closed fuel cycle strategy where plutonium is recycled. Presented calculations, according to moderate and high projections of nuclear energy development, confirm that plutonium recycling, although deployed to a limited extent, could be beneficial in reducing the stockpiles of nuclear spent fuel and in reducing the risks of proliferation due to the amount of fissile plutonium in the system. The improvement found in the consumption of natural uranium resources was limited promoting to this purpose the deployment of next-generation fast reactors. If a moderate development of nuclear energy is confirmed, the current capacity for reprocessing and MOX fuel fabrication could be sufficient to cope with the foreseen demand, on the contrary, significant investments could be necessary in case of steep increase of installed nuclear energy. Calculations were performed by means of the Dynamic Energy System – Atomic Energy code, a tool developed within the IAEA INPRO project.

14/02359 Waste heat recovery from the exhaust of a diesel generator using Rankine cycle

Hossain, S. N. and Bari, S. *Energy Conversion and Management*, 2013, 75, 141–151.

Exhaust heat from diesel engines can be an important heat source to provide additional power using a separate Rankine cycle (RC). In this research, experiments were conducted to measure the available exhaust heat from a 40 kW diesel generator using two 'off-the-shelf' heat exchangers. The effectiveness of the heat exchangers using water as the working fluid was found to be 0.44 which seems to be lower than a standard one. This lower performance of the existing heat exchangers indicates the necessity of optimization of the design of the heat exchangers for this particular application. With the available experimental data, computer simulations were carried out to optimize the design of the heat exchangers. Two heat exchangers were used to generate super-heated steam to expand in the turbine using two orientations: series and parallel. The optimized heat exchangers were then used to estimate additional power considering actual turbine isentropic efficiency. The proposed heat exchanger was able to produce 11% additional power using water as the working fluid at a pressure of 15 bar at rated engine load. This additional power resulted into 12% improvement in brake-specific fuel consumption (bsfc). The effects of the working fluid pressure were also investigated to maximize the additional power production. The pressure was limited to 15 bar which was constrained by the exhaust gas temperature. However, higher pressure is possible for higher exhaust gas temperatures from higher capacity engines. This would yield more additional power with further improvements in bsfc. At 40% part load, the additional power developed was 3.4% which resulted in 3.3% reduction in bsfc.