01 SOLID FUELS

Sources, winning, properties

14/01335 A novel technique for characterizing sintering propensity of low rank fuels for CFBC boilers

Lawrence, A. *et al*. *Fuel*, 2013, 109, 211–216.

In circulating fluidized bed combustion (CFBC) boilers, ash sintering may contribute to deposit formation in the cyclone, return leg and post-cyclone flue gas channel. In some cases, rapid sintering can lead to heavy agglomerate formation, which may finally inhibit circulation in dense phase areas (such as the seal pot). Hence, understanding the sintering behaviour before the fuel is used would be desirable for avoiding problems. Particle-to-particle sinter bonding usually results in shrinkage. The present technique is based on measuring the area shrinkage continuously during heating of ash pellets over a temperature range of interest. The area shrinkage measurement showed clear differences in the sintering profiles among the coal ashes tested. The present work describes the sintering profiles of ashes for the temperature range of 800–1100 °C. The fingerprint of sintering behaviour, over the temperature range, is made easy using the area shrinkage measurement. The probable mechanism behind the sintering behaviour observed in some low rank coals in the temperature range 800–1000 °C is proposed. The advantages over the other conventional techniques used for prediction of sintering such as compression strength measurement, electrical conductance are brought out.

14/01336 Application of gas chromatography/mass spectrometry in studies on separation and identification of organic species in coals

Fan, X. *et al*. *Fuel*, 2013, 109, 28–32.

The use of gas chromatography/mass spectrometry (GC/MS) in the investigation of coal structures and identification for composition of small molecules (with molecular weight at or less than 500 Da) was reviewed. Macromolecules and small molecules coexist in coals. Understanding the role of small molecules is fundamental for effective, clean and value-added utilization of coals. For coals after treatment (extraction, oxidation and liquefaction), small molecules can be extracted from the macromolecular network and analysed using GC/MS. Various kinds of organic species were identified using GC/MS, which gave explanation for coal structures and mechanisms for coal liquefaction and oxidation.

14/01337 Coal cleat permeability for gas movement under triaxial, non-zero lateral strain condition: a theoretical and experimental study

Perera, M. S. A. *et al*. *Fuel*, 2013, 109, 389–399.

As the permeability of coal seams is mainly determined by the network of natural fractures known as the cleat system, estimation of cleat permeability is of utmost importance for the carbon dioxide sequestration process in deep coal seams. The main objective of this study is to develop a new mathematical model for predicting cleat permeability under non-zero lateral strain conditions such as the conditions encountered in laboratory triaxial experiments. By applying the theory of elasticity to the constitutive behaviour of fractured rocks, a theoretical relationship between permeability and gas injecting pressure, confining pressure, axial load and gas adsorption in triaxial tests is developed. The new model was then verified using experimentally determined permeability data of two coal samples. Results indicate that the new model can fairly accurately predict the combined effects of effective stress and coal matrix swelling on cleat permeability for both CO_2 and N_2 injections at various injection pressures. The model also provides quite accurate prediction of the effect of confining pressure on cleat permeability for both CO_2 and N_2 injections. The model includes parameters for fractured rock properties, namely Poisson's ratio and Young's modulus. The model can be applied to predict cleat permeability, regardless of cleat size. When the accuracy of the new model is compared with the existing Gilman and Beckie model, with increasing injecting pressure both models show similar increments of N_2 permeability and different reductions for CO_2 permeability. This is due to the zero lateral strain assumption of the existing model, which is not applicable to the swelling process under triaxial test condition. The new model is more accurate for the prediction of CO_2 cleat permeability under triaxial test condition.

14/01338 Investigation on the macromolecular network structure of Xianfeng lignite by a new two-step depolymerization

Pan, C.-X. *et al*. *Fuel*, 2013, 109, 49–53.

Based on thermal extraction (TE) and mild oxidation, a new two-step depolymerization method was presented to investigate the macromolecular structure of Xianfeng lignite (XL). The TE of XL was carried out at 320 °C in 1-methylnaphthalene. The residue was oxidized with 5% H_2O_2 aqueous solution at 40 °C under normal nitrogen atmosphere for 4 h. Most of organic matter in XL was solubilized by the TE and subsequent oxidation. FTIR analysis reveals that the extract from the TE of XL is rich in aliphatic moieties and carbonyl groups but poor in aromatic rings and hydroxyl groups, whereas the residue is enriched in macromolecular aromatics. The mild oxidation introduced carbonyl groups into the macromolecular matrix of XL. The high yields of malonic acid and succinic acid and without benzene polycarboxlic acids from the residue oxidation suggest that $–CH_2–$ and $–CH_2CH_2–$ are main bridged bonds between aromatic rings and benzene ring should be an important aromatic ring in XL.

14/01339 Production and characterization of ash-free coal from low-rank Canadian coal by solvent extraction

Rahman, M. *et al*. *Fuel Processing Technology*, 2013, 115, 88–98.

In this work, ash-free coal (AFC) was extracted from low-rank Canadian coals with mean maximum vitrinite reflectance (MMVR) in the range of 0.38–0.69 using non-polar organic solvent, organic solvent combination (polar–non-polar solvent mixture), and with and without hydro-treated heavy aromatic hydrocarbon solvents from coal–tar industry to study the effect of type of coal and solvent type on the production yield of AFC. High temperature solvent extraction was carried out in 0.5 L autoclave in the temperature range of 473–723 K. It was observed that 1-methylnaphthalene (1-MN), a non-polar solvent did not give any significant difference in yields [~30% (daf)]. However, an extraction yield of 73% (daf) AFC was achieved using hydrotreated aromatic hydrocarbons at 673 K. The performance of extraction yields was correlated by the vitrinite content and MMVR of the coal and it was observed that higher proportions of vitrinite and a lower MMVR value of coal produced higher extraction yield. Proximate and ultimate analysis, FTIR, ICP-MS, ^{13}C CP/MAS NMR, thermogravimetric analysis and particle size distribution were used to characterize AFC. The heating value of the AFC was estimated to be in the range of 36–37 MJ/kg and a substantial decrease of sulfur content (*ca*. 12.5–61.1%) is also observed in AFC. AFC showed a narrower particle size distribution with a d_{50} of 7.0 μm.

14/01340 Thermochemical and combustion behaviors of coals of different ranks and their blends for pulverized-coal combustion

Moon, C. *et al*. *Applied Thermal Engineering*, 2013, 54, (1), 111–119.

In this research, a laboratory-scale slit burner, which accurately represents the conditions of a practical flame with a high heating rate and jet velocity, was used to study the combustion characteristics using thermal analysis. Results of thermogravimetric and differential thermal analyses (TGA and DTA) showed that low-rank coals influenced the ignition temperatures of blends whereas high-rank coals influenced their burnout temperatures. The first-order differential method was used to determine the kinetic parameters for coals of different ranks and their blends. Additionally, in pulverized-coal flames with CH* chemiluminescence band intensity, three reaction regions (zone I: preheating, zone II: volatile matter reaction and zone III: char reaction) were identified. The length of the reaction region and the mean flame temperature were found to be close to those for coal with a higher fuel ratio in zone I. In zone II, the fuel ratio influenced the length of the reaction region, but the mean flame temperature was closer to that for the low-rank coal and the maximum combustion reactivity shifted to a lower position. Moreover, the correlation between TGA and pulverized-coal flame was investigated. Based on the correlation, it was expected that prediction of the practical flame structure would be possible to some degree.

Preparation

14/01341 Adsorption of *Paenibacillus polymyxa* and its impact on coal cleaning

Abdel-Khalek, M. A. and El-Midany, A. A. *Fuel Processing Technology*, 2013, 113, 52–56.

The adsorption of microorganisms and bacteria on mineral surfaces depends mainly on the type of the bacteria used as well as the nature of the studied mineral surface. Such adsorption could change the surface properties of the mineral surface and leads to control its surface for increasing its separation selectivity from associated impurities or enhance/retard the adhesion with other substances. Therefore, in the current study, adsorption of *Paenibacillus polymyxa* on coal was studied. Several methods were used such as: zeta potential, adsorption isotherms, adsorption kinetics and Fourier transform infrared spec-

troscopy. The main goal is to determine the difference in surface behaviour of coal particles before and after the treatment with *P. polymyxa* bacteria. The results showed that electrostatic interactions are insignificant in *P. polymyxa* adsorption on coal particles. The results suggest that the adsorption of bacteria on the coal particles is mainly physical and it depends on electrostatic forces, hydrogen bonding as well as the hydrophobic forces between the bacteria wall and the organic matter in the coal and coal hydrophobicity.

14/01342 An optimization study of yield for a coal washing plant from Zonguldak region

Cebeci, Y. and Ulusoy, U. *Fuel Processing Technology*, 2013, 115, 110–114.

In this study, a coal washing plant in Zonguldak was optimized using equalization of incremental product quality approach which maximizes plant yield for a given ash constraint based on float–sink data. By maximization of yield using the software Solver for the identical elementary ash content and the specified ash level of 9.50%, the optimum cut points were determined for washing of the coarser size fraction (100–18 mm) and the finer size fraction (18–0.5 mm) by Drewboy Heavy Medium (HM) Bath and HM Cyclone, respectively. The results were compared with the plant operations in terms of product yield and ash content. Calculated yield percentage and ash percentage values with experimental yield percentage and ash percentage values from float–sink data of the used coal were also compared and they were in good agreement ($R^2 > 0.99$). By equalization of the incremental ash in order to get composite ash of 9.5%, the composite yield was maximized to 30.71% while the plant's yield was about 24.00%. This approach identified the optimum operating conditions for individual cleaning circuits as 1.693 and 1.682 for Drewboy HM Bath and HM Cyclone, respectively. It is worth pointing out that, this increase (6.71%) in the yield would be remarkable when considering the whole life of the washery and the annual production of the plant (about 700,000 tons). In addition, the yield was maximized to 33.41% for the target ash of 11.61% by similar optimization studies. The optimum operating cut points for HM Drewboy Bath and HM Cyclone was determined as 1.900 and 1.888, respectively. Yield optimization was also performed by taking $\alpha = 80$, which can be assumed ideal for HM separators. The results obtained by the two different calculations were very close to each other.

14/01343 Hierarchical porous carbons prepared from direct coal liquefaction residue and coal for supercapacitor electrodes

Zhang, J. *et al. Carbon*, 2013, 55, 221–232.

Hierarchical porous carbons were prepared from a coal liquefaction residue (CLR) and two coals, Shenhua (SH) coal with low and Shengli (SL) coal with high ash content, by KOH activation with the addition of some additives, and used as the electrode for supercapacitors. Two metal oxides (MgO and Al_2O_3) and three organic materials (sugar, urea and cetyltrimethylammonium bromide) were used as the additives, to investigate their effects on the structure and capacitive performance of the resultant carbons. The results show that the metal oxide and/or its salt formed by the reaction with KOH can serve as space fillers of nanopores in the carbonized carbon, while the gases produced by the decomposition of the organic additive can develop and/or widen some pores. Both help the carbon produced from CLR or the SH coal with low ash content to have additional mesopores and macropores, but destroy the structure of the carbon from the SL coal with high ash content. Compared with the carbon without any additive, the optimized hierarchical porous carbon with each additive shows a smaller equivalent resistance, much higher capacitance in a wide range of charge–discharge rates and excellent cycle stability when the carbon was used as supercapacitor electrode.

14/01344 Improved reactivity of large coal particles by K_2CO_3 addition during steam gasification

Coetzee, S. *et al. Fuel Processing Technology*, 2013, 114, 75–80.

In this study, the excess solution impregnation method was used to impregnate large coal particles (5 and 10 mm) with K_2CO_3, and the effect of the additive on steam gasification reactivity was investigated. A washed bituminous, medium rank-C Highveld coal, with an ash content of 12.6 wt% (air-dried basis), was used for experimentation. The excess solution method was used to impregnate coal particles with the selected additive, K_2CO_3, and results from XRF analysis indicated that the potassium loading increased from 0.05 wt% (raw coal) up to 0.83 wt% (impregnated coal), on a coal basis. The potassium-impregnated large coal particles were used for low temperature (800–875 °C) steam gasification experiments. Results obtained for the reactivity of the parent coal were compared to that of the impregnated coal, which indicated that the addition of K_2CO_3 increased the reaction rate of large coal particles by up to 40%. It was also found that the addition of K_2CO_3 decreased the activation energy, from 191 kJ/mol (raw coal) to 179 kJ/mol (impregnated coal).

14/01345 Increasing coal quality by oil agglomeration after ultrasonic treatment

Sahinoglu, E. and Uslu, T. *Fuel Processing Technology*, 2013, 116, 332–338.

In this study, oxidized and high-sulfur fine coal was subjected to oil agglomeration process after ultrasonic treatment. Power and time of ultrasonic treatment were selected as variable. Combustible recovery, ash rejection, pyritic sulfur rejection, ash separation efficiency and pyritic sulfur separation efficiency of the agglomeration process with and without ultrasonic treatment were determined. In addition, calorific value of the clean coal produced by agglomeration process was measured. In the agglomeration process without ultrasonic treatment, calorific value, combustible recovery, ash rejection and pyritic sulfur rejection were obtained to be 6518 kcal/kg, 63.78%, 75.19% and 92.64%, respectively. Ultrasonic treatment enhanced the performance of oil agglomeration process. By the application of ultrasonic treatment before agglomeration process, calorific value, combustible recovery, ash rejection and pyritic sulfur rejection were increased to maximally 6939 kcal/kg, 66.13%, 87.24% and 97.44%, respectively. In the study, changes on the surface structure of the coal after ultrasonic treatment were also examined. Particle breakage, formation of cracks and cavities, and altering of surfaces into fresh-clean surfaces were observed. Increase in time and power of ultrasonic treatment had slight positive effect on ash and pyritic sulfur rejections.

14/01346 Lignite upgrading by multi-stage fluidized bed pyrolysis

Zhou, Q. *et al. Fuel Processing Technology*, 2013, 116, 35–43.

This study is devoted to demonstrating experimentally the technical advantages of the multi-stage fluidized bed pyrolysis for upgrading lignite. A Chinese lignite was pyrolysed and partially gasified in a three-stage laboratory-scale fluidized bed, with an overflow standpipe between its neighbouring stages, to clarify the improvement on the pyrolysis product quality by increasing the number of the stages. While the bottom stage had the highest temperature of about 900 °C for fuel gasification, the upper stage had temperatures of 550–650 °C for coal pyrolysis. The multi-stage fluidized bed was operated with a continuous feed in the modes with one to three stages. The resulting yields of gas and tar were higher, whereas the yield of char was lower for the operations with multiple stages. The produced CO, H_2 and CH_4 in the two- and three-stage modes were more than that in the single-stage mode, having thus the higher gas heating value as well. The tar from the three-stage fluidized bed pyrolysis contained more light oil, and it plus phenol oil reached 99.5 wt% of the tar. The char produced in the multi-stage pyrolysis showed the higher thermal stability in terms of its higher ignition temperature and suppressed spontaneous combustion propensity.

Economics, business, marketing, policy

14/01347 An analysis of China's coal supply and its impact on China's future economic growth

Wang, J. *et al. Energy Policy*, 2013, 57, 542–551.

Many people believe that China's economic growth can continue almost indefinitely. For a manufacturing-based economy such as China's to continue to grow, it needs an adequate supply of inexpensive energy. To date, this energy growth has primarily come from coal, but China's indigenous coal supplies are now falling short of the amount needed to support this growth. In this situation, the status of China's future coal supply will be very important for China's future economic development. This analysis shows that China's ultimate recoverable coal reserves equal 223.6×10^9 MT, and its production will peak between 2025 and 2030, with peak production of approximately 3.9×10^9 MT. The extent to which China can import coal in the future is uncertain. With rising coal demand, this combination is likely to create a significant challenge to China's future economic development.

Derived solid fuels

14/01348 Assessment of the devolatilization behavior of fuel pellets in fluidized bed

Miccio, F. *et al. Fuel Processing Technology*, 2013, 115, 122–129.

The volatile release or devolatilization is an early stage occurring upon fuel particle feeding in a combustor. For coarse fuel particles, as in the case of fluidized bed (FB) combustion, it is mainly controlled by the thermal properties of the bed and fuel. The direct observation of the particle behaviour in fluidized bed is a simple and effective technique

for getting information on the devolatilization time and the number of volatile bubbles issuing from the fuel particle. The paper reports on experiments of devolatilization of different fuel particles of similar size, with particular concern on pellets composed by wood and wood/coal. The experimental technique was mainly based on the visual observation of the bed surface, the data-acquisition by a video-camera and the post-process elaboration of the frame sequences. Devolatilization times of dozens of seconds were measured for pelletized fuels, longer than those of normal wood particles. Two kinds of events were observed during devolatilization: (i) the eruption of a 'hot bubble' produced by bursting a submerged fuel-rich bubble and (ii) the generation of 'flames' at the bed surface. The number of such events was counted, obtaining values up to 100 per single particle under more critical conditions. A correlation between the number of monitored events and a dimensionless variable – function of FB and fuel properties – was proposed, providing a reasonable dependence on most relevant variables.

14/01349 Biochar-based catalyst for simultaneous reactions of esterification and transesterification

Dehkhoda, A. M. and Ellis, N. *Catalysis Today*, 2013, 207, 86–92.

Biochar, a by-product of fast pyrolysis of woody biomass, was developed as a renewable catalyst for simultaneous transesterification and esterification of canola oil and fatty acid (oleic acid) mixture at 150 °C under 1.52 MPa. Surface area and porosity of biochar were increased significantly from negligible to 990 m^2/g, and 0.9 cm^3/g through chemical activation method with KOH. The resultant biochar was sulfonated with fuming sulfuric acid to produce the biochar-based catalyst with high surface area and porosity (949 m^2/g and 0.85 cm^3/g). The ester formation yield was investigated based on the molar ratios of alcohol to canola oil (A : O), alcohol to oleic acid (A : FFA), or at constant mass ratio of alcohol to the mixture of oil and oleic acid. Increasing the FFA concentration from 15, 30 to 50 wt% (at constant A : O molar ratio) resulted in slight increase of reaction yields from 27.9, 35.1 to 36.7%, respectively. Results also revealed a continuous increase in reaction yield from 38.0 to 48.1% as increasing A : FFA molar ratio (from 10 : 1 to 30 : 1) at constant A : O. However, increasing A : O ratio (from 10 : 1 to 30 : 1) at constant A : FFA resulted in an unexpected decrease in the reaction yield from 48.1 to 28.8%. The biochar-based catalyst showed promising catalytic activity (48% yield in 3 h) for the combination of transesterification and esterification reactions in a mixture of canola oil and oleic acid for biodiesel production. Reaction yield decreased by ~8% on reusing the catalyst.

14/01350 Calcium-promoted catalytic activity of potassium carbonate for steam gasification of coal char: effect of hydrothermal pretreatment

Jiang, M. *et al. Fuel*, 2013, 109, 14–20.

Hydrothermal pretreatment of coal with the addition of $Ca(OH)_2$ was found more effective for promoting the K_2CO_3-catalysed char gasification than the physical addition way for both JY anthracite coal and HB bituminous coal used. The effect of hydrothermal pretreatment was more remarkable for JY coal which suffers significant catalyst deactivation due to its high mineral content. For this type of coal, employing more severe hydrothermal pretreatment conditions was proven to significantly enhance the gasification rate. It was observed that kaolinite and quartz in coal hydrothermally reacted with calcium forming hydrated calcium aluminosilicates, which, unlike the original minerals, was inactive for the deactivation reactions of potassium. Consequently, the hydrothermal pretreatment allowed more potassium to persist as a water-soluble entity during the gasification. This was a main mechanism underlying the promoted catalytic gasification by the hydrothermal treatment.

14/01351 Catalytic effects of Na and Ca from inexpensive materials on in-situ steam gasification of char from rapid pyrolysis of low rank coal in a drop-tube reactor

Zhang, L.-x. *et al. Fuel Processing Technology*, 2013, 113, 1–7.

Cost of catalysts is a crucial factor in realizing coal catalytic gasification process. In this study, inexpensive raw materials, soda ash (Na_2CO_3) and slaked lime ($Ca(OH)_2$), were selected as catalyst precursors, and Na-, Ca- and Ca/Na-loaded coals were prepared by an ion-exchange procedure using a sub-bituminous coal (Adaro coal, Indonesia). These coal samples were rapidly pyrolysed and *in situ* gasified in an atmospheric drop-tube reactor (DTR) at 850–1000 °C under a steam partial pressure of 0.05 MPa. The Na and Ca catalysts showed remarkable activity for gasification, and the Ca/Na-loaded coal exhibited the highest reactivity among the coal samples prepared. The char yield of the Ca/Na-loaded coal at 1000 °C was as low as 17.6 mol-C per 100 mol-C of coal, and more than 70% (on carbon basis) of its primary char was gasified within 3 s. At 900 °C, the coal with Ca-loading of 3.2 wt% showed catalytic activity higher than the coal with Ca-loading of 0.52 wt%. At 950 and 1000 °C, however, the coal with the lower Ca-loading showed higher activity. The XRD analysis suggested that the Ca catalyst with the lower loading was more resistant to coarsening along with the progress of char gasification.

14/01352 Effectiveness of crystallitic carbon from coal as milling aid and for hydrogen storage during milling with magnesium

Zhou, S. *et al. Fuel*, 2013, 109, 68–75.

This paper is concerned with the functions of crystallitic carbon, prepared from anthracite coal by demineralization and carbonization, for making Mg-based nanocomposites for hydrogen storage by reactive milling under hydrogen atmosphere. The TEM and XRD analysis show that in the presence of 30 wt% of crystallitic carbon, the Mg easily hydrided into β-MgH_2 of particle size 20–60 nm and crystal grain size 29.7 nm and a small amount of γ-MgH_2 after 3 h of milling under 1 MPa H_2. The hydrogen content of the composites is up to 5.81 wt% determined by water displacement method, and its dehydrogenation peak temperature is 344.2 °C by DSC analysis. The enthalpy and entropy changes of the hydrogen desorption reaction are 42.7 kJ/mol and 80.7 J/mol K, respectively, calculated by the van't Hoff equation from the p–C–T data in 300–380 °C. With the extension of milling time, more γ-MgH_2 yielded, and the endothermic peak of γ-MgH_2 separated from that of β-MgH_2. The C–H dangling bonds in the hydrogenated carbon were determined by FT-IR analysis. The dehydrogenation temperature of the materials decreased with the addition of Co, Ni, Fe and Al.

14/01353 Effects of petrochemical sludge on the slurry-ability of coke water slurry

Ma, X. *et al. Experimental Thermal and Fluid Science*, 2013, 48, 238–244.

The coke sludge slurry containing petroleum coke, petrochemical sludge, water and chemical additives was prepared to study effects of petrochemical sludge on its rheological properties and static stability characteristics. In the experiment, rheological properties of coke sludge slurry were investigated with rotational viscometer. The static stability characteristics were analysed by measuring the mass of the water separated from the slurry in a period. Effects of functional groups, inorganic minerals and surface structure on the slurry ability of coke sludge slurry were explored. The results suggest that coke water slurry which does not include petrochemical sludge is a dilatant fluid and petrochemical sludge can alter its rheological properties from shear thickening to shear thinning. As the petrochemical sludge amount is less than 6 wt% of petroleum coke in the coke sludge slurry, coke sludge slurry has similar rheological properties with coke water slurry; when the petrochemical sludge amount is 6 wt%, coke sludge slurry belongs to Newtonian fluid and turns into pseudo-plastic fluid after the petrochemical sludge amount exceeds 6 wt%. Besides, petrochemical sludge could improve the static stability characteristics of coke sludge slurry. Hydrophilic functional groups, inorganic minerals and surface structure of petrochemical sludge and petroleum coke play the key role on the rheological properties and static stability characteristics of coke sludge slurry.

14/01354 Potassium catalyzed CO_2 gasification of petroleum coke at elevated pressures

Malekshahian, M. and Hill, J. M. *Fuel Processing Technology*, 2013, 113, 34–40.

The rate of gasification can be increased by the addition of an alkali metal catalyst such as potassium. The effectiveness of potassium, however, depends on the characteristics of the feed material and the operating conditions. In this study, the effect of total pressure and partial CO_2 pressure on the gasification rate of K-impregnated petroleum coke was studied. Both raw petroleum coke and the produced char were impregnated with potassium carbonate at different loadings (0.03, 0.06, 0.10, 0.16 K/C molar ratio). The CO_2 gasification experiments were performed in a high-pressure thermogravimetric analyser at different temperatures (998–1098 K) and pressures (0.1–2.1 MPa), while the samples were characterized with Fourier transform infrared spectroscopy and inductively coupled plasma analysis. The rate increased with increasing pressure because of decreased catalyst volatilization and increased catalyst distribution. The determined activation energies at 0.1 MPa were 254 ± 21 and 133 ± 17 kJ/mol, for K-impregnated char and petroleum coke, respectively. The impregnation of potassium was more effective on raw petroleum coke because petroleum coke had more surface functional groups and a less ordered crystal structure than char.

14/01355 The role of density in the mechanical response of CNT turfs

Qiu, A. and Bahr, D. F. *Carbon*, 2013, 55, 335–342.

Solvent capillary and axial compression can be used to increase the density of as-grown vertically aligned carbon nanotube (CNT) arrays, herein referred to as turfs. During solvent evaporation, carbon nanotubes cluster together along their vertical growth axis, and axial

mechanical compression densifies through compressing tubes into tangled positions and decreasing the empty space between tubes in directions primarily perpendicular to the vertical growth axis. The elastic modulus of the turfs, measured by nanoindentation, is between four to 15 times higher after densification than that of pristine turfs and scales directly with densification ratio, while the adhesive properties remain unchanged. The electrical conductivity of the densified structure also scales with density. This suggests that multiple methods of post-growth modification of CNT arrays can achieve densified turfs with tailored mechanical properties without corresponding degradation of the electrical contact behaviour.

14/01356 Volatilization characteristics of solid recovered fuels (SRFs)

Montané, D. *et al. Fuel Processing Technology*, 2013, 113, 90–96.

The volatilization characteristics of three municipal solid waste (MSW)-derived materials (FO, RT and FL) produced by local waste-management companies were investigated as potential solid recovered fuels (SRFs). FL was prepared from sorted domestic waste and consisted of non-recyclable plastics, refuse paper and biomass. RT and FO were obtained through active hygienization of unsorted MSW and refuse materials from selective waste-collection streams. RT was rich in plastics and had low biomass, whereas FO was mainly biomass and refuse paper. The rate of energy release during volatilization depended on the content of biomass and plastic, especially at a low conversion. Major contaminants had different rates of volatilization. Nitrogen and sulfur tended to accumulate in the charred solid, and were released as SO_2 and nitrous oxides during both the volatilization–combustion stage and the char burning stage. Chlorine release was faster for the fuels rich in plastic waste. According to their ash melting characteristics and slagging indexes (1188 °C for FO, 1192 °C for RT and 1234 °C for FL) the three fuels were equivalent to commercial SRFs. The three fuels showed potential as standardized SRF, although it would be desirable to reduce their chlorine content and, in the case of FO, to increase its heating value.

14/01357 X-ray diffraction parameters and reaction rate modeling for gasification and combustion of chars derived from inertinite-rich coals

Everson, R. C. *et al. Fuel*, 2013, 109, 148–156.

An investigation was undertaken to determine the effect of carbon structural properties on the reactivity of chars derived from inertinite-rich coal. The structures of chars were characterized by X-ray diffraction and the reactivity evaluation with respect to gasification and combustion involving experimentation and reaction rate modelling was carried out. The effect of the aromaticity on the intrinsic reaction rates and associated activation energy for gasification and combustion of chars were determined based on chemical reaction rate controlled kinetics. Two sets of results were examined consisting of gasification with four char samples derived from different inertinite-rich coals prepared with a devolitalization temperature of 900 °C (set 1) and three chars from the same parent coal also rich in inertinites prepared at different devolitalization temperatures, namely 550, 700 and 850 °C (set 2). It was found that the aromaticity and fraction of crystalline carbon of the four chars prepared at the same temperature (set 1) varied in the ranges 0.85–0.95 and 0.52–0.72, respectively, and the chars prepared at different temperatures (set 2) in the ranges 0.82–0.92 and 0.44–0.74, respectively. The structural properties of the chars within each set of results were also very different which required reaction rate modelling for the determination of intrinsic reactivities. The random pore model with chemical reaction controlling described the reaction kinetics accurately and it was found that the intrinsic reactivity of the char decreased with increasing aromaticity while the activation energies decreased (aromaticity < 0.92) which indicated the effect of the variation of the distribution of aromatic/aliphatic structures on the intrinsic reaction rate. It is proposed that the aromaticity of chars be used as a predictive index for char reactivity under chemical reaction controlled conditions.

02 LIQUID FUELS

Sources, properties, recovery

14/01358 Effect of space distance for boiling heat transfer on micro porous coated surface in confined space

Liu, C.-F. and Yang, C.-Y. *Experimental Thermal and Fluid Science*, 2013, 50, 163–171.

This work provides an experimental analysis of the boiling heat transfer of methanol on plain and microporous coated surfaces inside confined space. Three space confinements with distance of 1.0, 2.0, 3.0 mm and an unconfined space were tested on plain and microporous coating surfaces. Effects of space confinement, surface treatment and heat flux on the heat transfer coefficient and critical heat flux were discussed. From the test results, it may be deduced that the boiling heat transfer performance in confined spaces was affected by four major effects, i.e. (a) vapour blowing and liquid suction effect, (b) thin-film evaporation, (c) vapour leaving resistance and (d) partial dryout effect on plain surface. But only (a) and (c) are important on microporous coating surface. The combination of these effects resulted in the microporous to plain surfaces heat transfer enhancement ratio to have different characteristics at low, moderate and high heat flux conditions. Microporous coating is a very effective boiling heat transfer enhancement treatment at low and moderate heat fluxes conditions. The enhancement ratio reduced in very narrow space confinement or at very high heat flux condition.

14/01359 Geochemical modelling of petroleum well data from the Perth Basin. Implications for potential scaling during low enthalpy geothermal exploration from a hot sedimentary aquifer

Wolff-Boenisch, D. and Evans, K. *Applied Geochemistry*, 2013, 37, 12–28.

Chemical analyses derived from petroleum exploration wells are notorious for their lack of key solute data and their potential to represent mixtures of reservoir and drilling fluids rather than pristine formation compositions. These drawbacks notwithstanding, they usually pose the only access to the reservoir geochemistry. Two literature protocols were applied to a dataset of incomplete major element analyses from 148 petroleum well samples from a database compilation of the Perth Basin whose deeper aquifers may serve as potential hot sedimentary aquifers for geothermal direct heat applications. The first protocol included a set of quality control criteria that reduced the number of relatively genuine formation well samples from the raw data pool by 71%. The remaining well analyses are invariably NaCl solutions of low to medium alkalinity and an ionic strength only occasionally reaching seawater salinity. The low amount of total dissolved solids indicates the absence of extended evaporites in the North Perth Basin and the prevalence of meteoric water infiltration and circulation at depths. The culled well samples underwent as a second protocol a forced equilibrium treatment to reconstruct *in situ* reservoir concentrations of missing elements (Si, Al, K), organic acid anions and non-carbonate alkalinity, and pH. The petroleum well samples were modelled to be in equilibrium with chalcedony (and kaolinite, albite and paragonite) in the reservoir which yielded better convergence than using quartz instead. The derived formation temperatures correspond to geothermal gradients in the majority of cases between 25 and 35 °C, in accord with literature findings. Those wells drilled to depth <1600 m returned questionably high geothermal gradients, an indication of incomplete mineral–fluid equilibrium. The measured pH (at ambient temperature) deviated in >90% of the wells from the calculated pH, either due to degassed CO_2 or unaccounted acetate alkalinity. The wells were further modelled to be undersaturated with respect to amorphous silica and anhydrite and not likely to experience scaling of any of these two phases during geothermal production at depth <3800 m. For calcite, scaling predictions depend in how far bubbling and phase segregation can be suppressed. For the six different stratigraphies investigated here, calculated bubble points were low, indicating that pressurization of the entire production and re-injection line seems viable. Based on a calcite growth model from the literature it is shown that, if bubble formation and concomitant carbonate flash scaling cannot be averted, the production well should be as shallow as the temperature requirements of the geothermal production allow for. This study promotes the application of readily accessible protocols and a scaling model to deep well samples that may otherwise appear to have little geochemical value because of the way the samples were collected and handled. After data culling and treatment, insights into the geochemistry and scaling potential of deep clastic formations of the North Perth Basin that may hold the potential for geothermal exploitation as hot sedimentary aquifers can be gained.

14/01360 Oil recovery mechanisms and asphaltene precipitation phenomenon in immiscible and miscible CO_2 flooding processes

Cao, M. and Gu, Y. *Fuel*, 2013, 109, 157–166.

In this paper, oil recovery mechanisms and asphaltene precipitation phenomenon of immiscible and miscible CO_2 flooding processes in the tight sandstone reservoir core plugs are experimentally studied. First, the vanishing interfacial tension (VIT) technique is applied to determine the minimum miscibility pressure (MMP) between the original light crude oil and CO_2. Second, a total of five coreflood tests are performed at the actual reservoir temperature. It is found that the oil recovery factor (RF) increases monotonically as the injection

pressure increases during the immiscible CO_2 flooding. The increased oil RF is attributed to the increased CO_2 solubility in oil, reduced oil viscosity, increased CO_2 viscosity, and reduced equilibrium interfacial tension (IFT) of the light crude oil–CO_2 system. Once the injection pressure exceeds the MMP, the oil RF increases slightly and will reach an almost constant maximum value. In this case, it is the multi-contact miscibility (MCM) and the extremely low equilibrium IFT that jointly make the ultimate oil RF high and unchanged. Moreover, the oil RF after CO_2 breakthrough (BT) increases slightly in the immiscible case but substantially in the miscible case. This is due to the strong light-hydrocarbons extraction by CO_2 and the miscible displacement in the second case. On the other hand, the measured average asphaltene content of the produced oil and the measured oil effective permeability reduction are found to be higher in the immiscible flooding process. They both reach some lower values in the miscible case. Finally, the experimental results obtained in this study at the actual reservoir temperature of $T_{res} = 53.0\,^{\circ}C$ are compared with those attained previously at the laboratory temperature of $T_{lab} = 27.0\,^{\circ}C$ to examine the temperature effect on the CO_2-based oil recovery process.

Transport, refining, quality, storage

14/01361 Beneficial effects of polycyclic aromatics on oxidative desulfurization of light cycle oil over phosphotungstic acid (PTA) catalyst

Yun, G.-N. and Lee, Y.-K. *Fuel Processing Technology*, 2013, 114, 1–5.

The amphiphilic phosphotungstic acid catalyst (A-PTA) was prepared with quaternary ammonium salt to apply for the oxidative desulfurization (ODS) of light cycle oil (LCO), resulting in high activity of the ODS conversion of 95%, at H_2O_2/S ratio of 10 and 353 K. The model reaction tests for the ODS of refractory sulfur compounds in n-octane demonstrated that the addition of indole drastically reduced overall ODS conversion, while the introduction of 1-methylnaphthalene fully recovered the ODS activity, which were attributed to the high solubility of the oxidized S or N compounds in the two-ring aromatics.

14/01362 Combining coal gasification, natural gas reforming, and external carbonless heat for efficient production of gasoline and diesel with CO_2 capture and sequestration

Salkuyeh, Y. K. and Adams II, T. A. *Energy Conversion and Management*, 2013, 74, 492–504.

In this paper, several novel polygeneration systems are presented which convert natural gas, coal, and a carbonless heat source such as high-temperature helium to gasoline and diesel. The carbonless heat source drives a natural gas reforming reaction to produce hydrogen-rich syngas, which is mixed with coal-derived syngas to produce a syngas blend ideal for the Fischer–Tropsch reaction. Simulations and techno-economic analyses performed for 16 different process configurations under a variety of market conditions indicate significant economic and environmental benefits. Using a combination of coal, gas and carbonless heat, it is possible to reduce CO_2 emissions (both direct and indirect) by 79% compared to a traditional coal-to-liquids process, and even achieve nearly zero CO_2 emissions when carbon capture and sequestration technology is employed. Using a carbonless heat source, the direct fossil fuel consumption can be reduced up to 22% and achieve a carbon efficiency up to 72%. Market considerations for this analysis include prices of coal, gas, high-temperature helium, gasoline, and CO_2 emission tax rates. The results indicate that coal-only systems are never the most economical choice, unless natural gas is more than \$5/MMBtu.

14/01363 Demonstration test result of high pressure acid gas capture technology (HiPACT)

Tanaka, K. *et al. Energy Procedia*, 2013, 37, 461–476.

High-pressure acid-gas capture (HiPACT) technology is an advanced CO_2 capture technology that contributes to economical carbon dioxide capture and storage (CCS) implementation. A demonstration test was conducted in INPEX's Koshijihara natural gas plant in Japan. HiPACT showed excellent performance in CO_2 absorption; 20–27% reduction of solvent circulation rate and 10–20% savings in reboiler duty compared with OASE purple were achieved, keeping the CO_2 specification at the absorber overhead unaffected. A case study suggests that HiPACT reduces CO_2 recovery cost (AGRU + CO_2 compressor) by 25–35% over OASE purple.

14/01364 Design and off-design simulations of combined cycles for offshore oil and gas installations

Nord, L. O. and Bolland, O. *Applied Thermal Engineering*, 2013, 54, (1), 85–91.

Combined cycles applied on offshore oil and gas installations could be an attractive technology on the Norwegian continental shelf to decrease costs related to CO_2 emissions. Current power plant technology prevailing on offshore oil and gas installations is based on simple cycle gas turbines for both electrical and mechanical drive applications. Results based on process simulations showed that net plant efficiency improvements of 26–33% (10–13%-points) compared to simple cycle gas turbines can be achieved when the steam-bottoming cycles are designed for compactness and flexibility. The emitted CO_2 could be decreased by 20–25% by opting for a combined cycle rather than a simple cycle gas turbine. A clear disadvantage for offshore applications is that the weight-to-power ratio was 60–70% higher for a compact combined cycle than for a simple cycle gas turbine based on results in this study. Once-through heat recovery steam generator technology can be an attractive option when designing a steam bottoming cycle for offshore applications. Its flexibility, the avoidance of steam drums, and, with the right material selection, the possibility to avoid the bypass stack while allowing for dry heat recovery steam generator operation are all advantages for offshore applications. All process models, that were developed for offshore installations in the study presented, included once-through technology. A combined cycle plant layout for an offshore installation with both mechanical drive and generator drive gas turbines was included in the study. This setup allows for flexibility related to changes in demand for both mechanical drive and electricity. With the selected setup, designed for 60 MW shaft power, demand swings of approximately ± 10 MW could be handled for either mechanical drive or electrical power while keeping the other drive-mode load constant.

14/01365 DSC study on combustion and pyrolysis behaviors of Turkish crude oils

Kok, M. V. and Gundogar, A. S. *Fuel Processing Technology*, 2013, 116, 110–115.

This study investigated the non-isothermal thermal behaviour and kinetics of Turkish crude oils under combustion and pyrolysis conditions using differential scanning calorimetry (DSC). On DSC combustion curves, two exothermic oxidation regions were detected known as low temperature (LTO) and high temperature oxidation (HTO). Again, two distinct reaction regions were revealed under pyrolysis conditions and DSC curves exhibited endothermic behaviour for both the distillation and cracking regions. In consequence of thermal analyses, the heat of reaction amount was related to the °API gravity and accordingly to the asphaltene content of crude oils. It was proved that, with the decrease in °API gravity of crude oil, its heat release during HTO and heat requirement for cracking reaction increase. Experimental results showed that the reaction temperature intervals, peak temperatures and heat flows shifted to greater degrees for higher heating rates. With the application of ASTM I–II and Roger & Morris kinetic methods, it was observed that heavier oils with higher asphaltene content had greater activation energy and Arrhenius constant values.

14/01366 Microcosm assessment of the biogeochemical development of sulfur and oxygen in oil sands fluid fine tailings

Chen, M. *et al. Applied Geochemistry*, 2013, 37, 1–11.

Bitumen recovery from Alberta oil sands generates fluid fine tailings, which are retained in tailings ponds where solids settle and release process water. The recovered water is recycled for bitumen extraction, while the resulting tailings are incorporated into various landforms for reclamation, with one option being conversion of tailings basins to viable end pit lakes. Tailings ponds commonly host diverse microbial communities, including SO_4-reducing prokaryotes. The highly reducing nature of the hydrogen sulfide produced by these prokaryotes may impact the biogeochemical cycling of key nutrients. However, the behavioural dynamics of hydrogen sulfide production in ponds containing fluid fine tailings remain to be clearly explained. In this study, microcosms are used as analogues of the sediment–water interface of a tailings pond undergoing reclamation to determine sulfide generation patterns and the behaviour of O_2. In the microcosms, hydrogen sulfide fluxes correlated positively with biotic activity, reaching levels of over 2×10^3 nmol cm^{-2} s^{-1}, leading to Fe sulfide formation. Depth-related hydrogen sulfide profiles in the microcosms were comparable to those encountered *in situ*, in Syncrude's West In-Pit, an active tailing pond. Oxygen diffusion across the fluid fine tailing sediment–water interface was controlled to different degrees by both biotic and abiotic processes. The results have implications for quantitatively estimating the impact of hydrogen sulfide production, O_2 availability, and biogeochemical cycling of key nutrients important for the success of life in fluid fine tailings-affected ecosystems. This paper shows that this production of hydrogen sulfide may be a self-limiting process, which will begin to decrease after a period of time.

14/01367 Mitigation of crude oil fouling by turbulence enhancement in a batch stirred cell

Yang, M. *et al. Applied Thermal Engineering*, 2013, 54, (2), 516–520.
A compact batch stirred cell has been used to investigate crude oil fouling on bare mild steel test probes and on similar probes fitted with thin wires to promote turbulence and increase surface shear stresses. The results show that, under otherwise identical operating conditions, the fouling rate on the surface of the probe fitted with wires was significantly lower than on the surface of the bare probe. Moreover, the fouling resistance data using the wired probe were seen to be much more scattered over time which suggests that the additional turbulence, and hence the associated additional shear stress, and perhaps even the associated uneven circumferential shear stress distribution, were creating a greater random removal of the fouling deposit from the surface. Computational fluid dynamic (CFD) simulations of the fluid flow for both the bare and wired probes were conducted using the commercial multiphysics package Comsol 4.2. The CFD simulation results show that the surface shear stress indeed varies in a periodic manner around the wired probe surface, being greater immediately in front of a wire, and lower immediately behind a wire in respect of the flow direction. The CFD simulation results show that, for otherwise identical conditions, the shear stress on the wired probe was significantly greater than that on original bare probe even at the point of lowest circumferential shear stress. The CFD results thereby allow better interpretation of the experimental fouling data on the enhanced surface.

14/01368 Reducing heat loss of fluids in heavy oil wellbore using two-phase closed thermosyphon sucker rod

Zhang, X. and Che, H. *Energy*, 2013, 57, 352–358.
The purpose of the research is to verify the viability and the applicability of two-phase closed thermosyphon (TPCT) sucker rod in a cyclic steam stimulation for heavy oils. On the basis of the previous research and the basic principles of TPCT, the laboratory experiment system was set up and the heat-transfer experiment was conducted using liquid ammonia as the working fluid. The laboratory data show that the TPCT sucker rod can use the heat energy from hot water depending on the vaporization and condensation of ammonia to transfer heat. Based on the results from the laboratory experiment, the site application of the TPCT sucker rod was undertaken in well H127–26–34 of the Liaohe oilfield in China. The site application results demonstrate that the TPCT sucker rod can decrease the heat loss of fluids in wellbore and improve well performance during cyclic steam stimulation.

14/01369 Research on the MgO-supported solid-base catalysts aimed at the sweetening of hydrogenated gasoline

Zhang, Y. *et al. Fuel Processing Technology*, 2013, 115, 63–70.
The gas–liquid–solid heterogeneous base-catalysed oxidation of n-octane thiol and tert-butyl thiol by molecular oxygen was investigated. The activity and stability of MgO-supported NaOH and monometallic Cu, Ni as well as bimetallic Cu–Ni catalysts were studied. The catalysts were further characterized by XRD, FT-IR, XPS and EPR. Compared with commercial cobalt phthalocyanine catalyst (CoPc catalyst), the MgO-supported bimetallic Cu–Ni catalyst displayed an enhanced stability to the oxidation of iso-mercaptan, and the catalytic lifetime is 10 h longer than that of CoPc catalyst. It is found that the superoxide anions result from defects and small crystalline size play an important role in conversion of the iso-mercaptans, the more the lattice distortion, the higher the amount of surface adsorbed oxygen, the better was the performance of the sweeten-catalyst. Moreover, compared with commercial CoPc catalyst, the NaOH-rich catalyst is more resistant to deactivation of the oxidation of long chain thiol, and the catalytic lifetime is 26 h longer than that of CoPc catalyst. The superbasicity of the NaOH-rich catalyst is responsible for the formation of mercaptide ion, which is the rate-controlling step for the oxidation of long-chain thiol. The mercaptans of different structures conform to different reaction mechanisms.

14/01370 Synergistic effect of alkyl-O-glucoside and -cellobioside biosurfactants as effective emulsifiers of crude oil in water. A proposal for the transport of heavy crude oil by pipeline

Cerón-Camacho, R. *et al. Fuel*, 2013, 110, 310–317.
Alkyl-O-glucoside and alkyl-O-cellobioside biosurfactants were synthesized with a long fatty chain (C_8–C_{18}) in order to prepare stable and low viscous oil-in-water (O/W) emulsions of a Mexican heavy crude oil. The resulting O/W emulsions, prepared with a single alkyl-O-glucoside or alkyl-O-cellobioside, were very unstable and broke out. Only the use of tetradecyl-O-cellobioside allowed the formation of a poor stable complex emulsion with the broader particle size distribution and more viscous than other emulsions. Nonetheless, a synergistic effect was observed when a biosurfactant mixture was used and the resulting emulsions were stable for several days while water separation occurred constantly within 40 days in static conditions. The mixture of biosurfactants with a pC_{20} value higher than 4.0 and a CMC/C_{20} ratio higher than 1.0 favoured the formation of a less viscous, narrow particle size distribution and thermal stable O/W emulsion. This feature is important when considering the pipeline transportation of heavy and extra-heavy crude oils as O/W emulsions. The authors present the characterization of biosurfactants as well as the formulation and properties of O/W emulsions of a Mexican heavy crude oil.

14/01371 Toward an intelligent approach for determination of saturation pressure of crude oil

Farasat, A. *et al. Fuel Processing Technology*, 2013, 115, 201–214.
Bubble point pressure is a crucial PVT parameter of reservoir fluids, which has a significant effect on oil field development strategies, reservoir evaluation and production calculations. This communication presents a new mathematical model to calculate the saturation pressures of crude oils as a function of temperature, hydrocarbon and non-hydrocarbon reservoir fluid compositions, and characteristics of the heptane-plus fraction. The model was developed and tested using a total set of 130 experimentally measured compositions and saturation pressures of crude oil samples from different geographical locations covering wide ranges of crude oil properties and reservoir temperatures. In-depth comparative studies have been carried out between this new model and five well known predictive models for estimation of saturation pressure of crude oils. The results show that the developed model is more accurate and reliable with the average absolute relative deviation of 4.7% and correlation coefficient of 0.992. In addition, it is shown that the proposed model correctly captures the physical trend of changing the saturation pressure as a function of the input variables. Finally, the applicability domains of the proposed model and quality of the existing experimental data were examined by outlier diagnostics.

14/01372 Upgrading fast pyrolysis liquids: blends of biodiesel and pyrolysis oil

Alcala, A. and Bridgwater, A. V. *Fuel*, 2013, 109, 417–426.
Fast pyrolysis liquid or bio-oil has been used in engines with limited success. It requires a pilot fuel and/or an additive for successful combustion and there are problems with materials and liquid properties. It is immiscible with all conventional hydrocarbon fuels. Biodiesel, a product of esterification of vegetable oil with an alcohol, is widely used as a renewable liquid fuel as an additive to diesel at up to 20%. There are however limits to its use in conventional engines due to poor low temperature performance and variability in quality from a variety of vegetable oil qualities and variety of esterification processes. Within the European Project Bioliquids-CHP – a joint project between the European Commission and Russia – a study was undertaken to develop small-scale CHP units based on engines and microturbines fuelled with bioliquids from fast pyrolysis and methyl esters of vegetable oil. Blends of bio-oil and biodiesel were evaluated and tested to overcome some of the disadvantages of using either fuel by itself. An alcohol was used as the co-solvent in the form of ethanol, 1-butanol or 2-propanol. Visual inspection of the blend homogeneity after 48 h was used as an indicator of the product stability and the results were plotted in a three phase chart for each alcohol used. An accelerated stability test was performed on selected samples in order to predict its long-term stability. It was concluded that the type and quantity of alcohol is critical for the blend formation and stability. Using 1-butanol gave the widest selection of stable blends, followed by blends with 2-propanol and finally ethanol, thus 1-butanol blends accepted the largest proportion of bio-oil in the mixture.

Economics, business, marketing, policy

14/01373 Industrial structure and oil consumption growth path of China: empirical evidence

Zheng, Y. and Luo, D. *Energy*, 2013, 57, 336–343.
The relationships between industrial structure and the respective growth paths of oil consumption of the primary, secondary and tertiary industries in China are examined. Based on the results, the degrees of grey correlations between total oil consumption and output values of the primary and secondary industries in China have declined, whereas that between Chinese oil consumption and output values of tertiary industries has increased. Using the vector-error correction model, the long- and short-run relationships between oil consumption and the three types of industries are identified. From 1978 to 2009, the long-run elasticity of total oil consumption with respect to the output value of tertiary industries ranked first, followed by the secondary industries. The negative effects of the primary industries on total oil consumption result from the 'crowding out effects' of the two other industries. Although the error correction coefficients are small, the short-term impacts of the inhibition of oil consumption are limited, and China's oil consumption growth shows strong continuity and inertia. Causal tests

and co-integration show that output values of the three types of industries Granger cause total oil consumption in the long run but not in the short run.

14/01374 Iran's oil development scenarios by 2025

Abbaszadeh, P. *et al. Energy Policy*, 2013, 56, 612–622.

Energy resources in Iran consist of the fourth largest oil reserves and the second largest natural gas reserves in the world. At present, due to political reasons, the investment trend is not particularly positive. Based on the Fifth Development Strategy, Iran needs $200 billion of investment in the country's first industry (i.e. oil), and given the objectives of the perspective document, the Iran needs more than $500 billion investment during the next 15 years. This paper examined Iran's energy status. Oil future scenarios, which have been developed by the research centre of the Iranian parliament, have also been analysed. Four scenarios that express different modes of production and consumption are developed, namely: Thunder, Behemoth, Snowman, and Poor Addict. Finally, a comprehensive analysis for achieving the secure and sustainable future on the geopolitical, geo-economic and geocultural situation is presented.

14/01375 Jump dynamics in the relationship between oil prices and the stock market: evidence from Nigeria

Fowowe, B. *Energy*, 2013, 56, 31–38.

This study investigates the relationship between oil prices and returns on the Nigerian stock exchange. By using GARCH-jump models, the volatility of stock returns can be modelled and the effect of extreme news events on returns can be taken into account. The empirical results show a negative but insignificant effect of oil prices on stock returns in Nigeria. Possible explanations for this result could be because the stock exchange is dominated by the banking sector and there are too few oil-related firms to warrant a channelling of high oil prices to the stock market; or because of the high transactions costs on the stock exchange which discourages investment; or because of low liquidity on the stock exchange.

14/01376 Natural gas supply stability and foreign policy

Shaffer, B. *Energy Policy*, 2013, 56, 114–125.

This article studies factors that affect stability of supply of natural gas. It examines the relative influence of political relations between the involved states on the stability of supply. The article identifies the factors that affect the propensity of a state to use disruption of natural gas supply in order to promote foreign policy goals. The article is based on the study of 35 supply relations and two case studies. The article claims that disruption of supplies can be initiated not only by supplier states, but transit and consumer states. It claims that natural gas supply relations generally take three forms: neither side is dependent on the gas trade, one side is dependent on the gas trade, or the sides are interdependent in the gas trade. Cases of significant asymmetry of the degree of dependence in the gas trade are most likely to be exploited by the less dependent party for foreign policy gain. The article claims that the prevailing political relations between gas trading states are only one of the factors affecting the stability of supply.

14/01377 Reform of refined oil product pricing mechanism and energy rebound effect for passenger transportation in China

Lin, B. and Liu, X. *Energy Policy*, 2013, 57, 329–337.

Improving energy efficiency is the primary method adopted by the Chinese government in an effort to achieve energy conservation target in the transport sector. However, the offsetting effect of energy rebound would greatly reduce its real energy-saving potentials. The authors set up a linear approximation of the almost ideal demand system model to estimate the rebound effect for passenger transportation in China. Real energy conservation effect of improving energy efficiency can also be obtained in the process. The result shows that the rebound effect is approximately 107.2%. This figure signifies the existence of 'backfire effect', indicating that efficiency improvement in practice does not always lead to energy saving. The authors conclude that one important factor leading to the rebound effect, is the refined oil pricing mechanism. China's refined oil pricing mechanism has been subjected to criticism in recent years. The results of simulation analysis show that the rebound could be reduced to approximately 90.7% if the refined oil pricing mechanism is reformed. In this regard, further reforms in the current refined oil pricing mechanism are suggested.

14/01378 Symmetric or asymmetric oil prices? A meta-analysis approach

Perdiguero-García, J. *et al. Energy Policy*, 2013, 57, 389–397.

The analysis of price asymmetries in the gasoline market is one of the most widely studied in energy economics. However, the great variation in the outcomes reported makes the drawing of any definitive conclusions difficult. Given this situation, a meta-analysis serves as an excellent tool to discover which characteristics of the various markets analysed, and which specific features of these studies, might account for these differences. In adopting such an approach, this paper shows how the particular segment of the industry analysed, the characteristics of the data, the years under review, the type of publication and the introduction of control variables might explain this heterogeneity in results. The paper concludes on these grounds that increased competition may significantly reduce the possibility of occurrence of asymmetric behaviour. These results should be taken into consideration therefore in future studies of asymmetries in the oil industry.

Derived liquid fuels

14/01379 Coal-derived liquid asphaltenes diffusion and adsorption in supported hydrotreating catalysts

Roussi, L. *et al. Fuel*, 2013, 109, 167–177.

Hindered diffusion and adsorption phenomena of coal asphaltenes inside the porous network of hydrotreating catalysts are discussed in this paper. After solvent extraction from a coal-derived liquid and solubilization in THF, asphaltenes were contacted with a series of mesoporous hydrotreating catalysts and adsorption–diffusion phenomena recorded by UV–Vis spectroscopy measurements. The effect of the porosity of various NiMo(P) catalysts supported on monomodal mesoporous or bimodal (meso–macro) alumina carrier was investigated. The parameters estimations have been performed, discussed and those obtained with the bimodal (meso–macro) alumina catalyst have been compared to petroleum asphaltenes data. The range of studied concentrations corresponds to cluster formation domain. The results evidence that coal asphaltenes aggregates are smaller, have lower molecular weight and exhibit a much higher diffusion coefficient than petroleum asphaltene aggregates. These results bring important insights for the interpretation of the performance of the catalysts during coal-derived liquid upgrading. Concerning adsorption phenomena, the adsorption constants of coal asphaltenes and petroleum asphaltenes have been found equivalent. The adsorption saturation concentration of coal asphaltenes is higher than that of petroleum asphaltenes. The effective diffusion coefficients obtained at ambient temperature were correlated to the catalytic performances observed during coal-derived liquid hydrotreatment. It points out that the conversion of coal-derived liquid into the porous network of this catalyst is a hindered phenomenon, and that pore size distribution of the support has a great influence on the hydroliquefaction efficiency.

14/01380 Comparative studies of thermochemical liquefaction characteristics of microalgae, lignocellulosic biomass and sewage sludge

Huang, H.-j. *et al. Energy*, 2013, 56, 52–60.

Lignocellulosic biomass, microalgae and sewage sludge have distinct compositions and structures to each other. To understand the effect of feedstock differences on biomass liquefaction process, the liquefaction characteristics of rice straw (lignocellulosic biomass), *Spirulina* (microalgae) and sewage sludge were comparatively studied. Liquefaction experiments were performed in a 500 mL autoclave at identical conditions (623 K, 9.4–10.1 MPa and 20 min retention time). Although the content of organic materials in sewage sludge was the lowest among above three biomasses, the yield of bio-oil from sewage sludge reached up to $39.5 \pm 1.16\%$, higher than those from rice straw ($21.1 \pm 0.93\%$) and *Spirulina* ($34.5 \pm 1.31\%$). Besides, the bio-oils from sewage sludge had the highest heating value (36.14 MJ/kg). However, *Spirulina* showed the highest conversion ($79.7 \pm 1.02\%$). GC–MS analysis results indicated that the major compounds in the bio-oil from rice straw were phenolic compounds. In case of sewage sludge and *Spirulina*, esters were the main compositions. The volatility distribution of hydrocarbons was evaluated by C-NPgram (carbon-normal paraffin gram). It was showed that the majority of hydrocarbons from sewage sludge and *Spirulina* were distributed at C_{17} and C_{20}, whereas they were distributed at C_8 in rice straw-derived bio-oil. The types of feedstocks have a significant effect on biomass liquefaction.

14/01381 Development of oxazolidines derived from poly*iso*butylene succinimides as multifunctional stabilizers of asphaltenes in oil industry

Mena-Cervantes, V. Y. *et al. Fuel*, 2013, 110, 293–301.

The aim of this research was to develop novel multifunctional stabilizers of asphaltenes (Asph) for the control of fouling in different stages of petroleum industry. Novel stabilizers were obtained from the reaction between poly*iso*butenyl succinic anhydride (PIBSA), 2-(2-aminoethylamino)ethanol (AEAE) and an R-substituted aldehyde, resulting in three 2-R-(poly*iso*butylenesuccinimidyl)oxazolidines as prototypes of multifunctional Asph stabilizers, where R is –H (P1), $-C_5H_{11}$ (P2) or *–ortho*$(OH)C_6H_4$ (P3). Compounds P1–3 were characterized by FTIR, ^1H, ^{13}C and 2D NMR spectroscopies, and

assessed in four different types of evaluations: (i) Asph dispersion by UV–vis, (ii) displacement of Asph onset precipitation, at ambient conditions, (iii) inhibition of electric field induced deposition of Asph and (iv) displacement of Asph onset precipitation, at reservoir conditions. All the latter individual efficiencies were included in a multifunctional development factor (MDF) resulted in 0.626 for P1, 0.326 for P2 and 0.679 for P3, where the higher value corresponded to the highest efficiency. For comparison purposes, two commercial stabilizers of Asph were also evaluated, resulting in MDF of 0.012 and 0.162, being P1–3 clearly better multifunctional chemicals. Best novel prototype was selected for industrial evaluation by taking into account technical and economic criteria, thus P1 compound was chosen as active component of DAIM chemical and was successfully assessed at industrial scale in a production well of Petróleos Mexicanos to control Asph fouling. The continuous injection of DAIM produced important benefits to the oil well productivity, such as the decrease of the frequency of cleaning operations from 11 to 4 in a 1-year evaluation period and the reduction of production rate decay from −1.48 to $-0.032\,m^3$/day, *ca.* 46 times less in comparison when the well was operated without Asph stabilizer.

14/01382 Diesel steam reforming: comparison of two nickel aluminate catalysts prepared by wet-impregnation and co-precipitation

Achouri, I. E. *et al. Catalysis Today*, 2013, 207, 13–20.

γ-Al_2O_3 supported Ni–Al spinel catalysts, prepared by co-precipitation and wet impregnation, were produced, analysed and tested on commercial diesel steam reforming. The study of the preparation method's effect on the catalytic activity, builds on a previously patented Ni–Al spinel ($NiAl_2O_4$) catalyst supported on alumina (Al_2O_3) and yttria-stabilized zirconia (YSZ). This non-noble metal-based $NiAl_2O_4$/Al_2O_3–YSZ catalyst demonstrated high activity for commercial diesel and biodiesel steam reforming. Diesel steam reforming experiments were performed in a fixed-bed reactor setup, with a proprietary diesel–water emulsion mixture at 760 °C. The two tested catalytic formulations yielded the same overall conversion while the products obtained were significantly different. Thus, the catalyst produced via the co-precipitation method (Copr): (a) suffered rapid deactivation from carbon deposition; (b) produced five times more methane than the catalyst produced via the wet impregnation method (Impr) and (c) showed a decreasing hydrogen production. The Impr catalyst exhibited a higher stability for diesel steam reforming with no signs of carbon formation or activity loss. The difference between Impr and Copr catalyst activities is related to the Ni-aluminates dispersion: located on the surface for the Impr catalyst, whereas located in the bulk of the Copr catalyst. In order to correlate their activities to their physicochemical properties, both new catalytic formulations presented in this work were characterized before and after steam reforming tests, using scanning electron microscopy, X-ray diffraction, as well as temperature programmed reduction.

14/01383 Diesel-like hydrocarbon production from hydroprocessing of relevant refining palm oil

Kiatkittipong, W. *et al. Fuel Processing Technology*, 2013, 116, 16–26.

This paper demonstrates the initiated use of relevant refining palm oil for bio-hydrogenated diesel production. The conversions of crude palm oil (CPO) and its physical refining including degummed palm oil (DPO) and palm fatty acid distillate (PFAD) to diesel fuel by hydroprocessing were studied. The effects of operating parameters (i.e. reaction time, operating temperature, and pressure) and catalyst (i.e. Pd/C and NiMo/γ-Al_2O_3) were examined in order to determine suitable operating condition for each feedstock. It was found that the hydroprocessing of CPO with Pd/C catalyst at 400 °C, 40 bar and reaction time of 3 h provides the highest diesel yield of 51%. When gum which contains phospholipid compounds is removed from CPO, namely DPO, the highest diesel yield of 70% can be obtained at a shorter reaction time (1 h). In the case of PFAD, which consists mainly of free fatty acids, a maximum diesel yield of 81% could be observed at milder conditions (375 °C with the reaction time of 0.5 h). The main liquid products are *n*-pentadecane and *n*-heptadecane, having one carbon atom shorter than the corresponding fatty acids according to decarboxylation/decarbonylation pathways. Pd/C catalyst shows good catalytic activity for fatty acid feedstocks but becomes less promising for triglyceride feedstocks when compared to NiMo/γ-Al_2O_3.

14/01384 Dynamic cyclical comovements between oil prices and US GDP: a wavelet perspective

Benhmad, F. *Energy Policy*, 2013, 57, 141–151.

This study uses wavelet analysis to investigate the cyclical co-movements between crude oil prices and US gross domestic product (GDP), taking into account the decline in the volatility of US GDP growth that has occurred since the mid-1980s. The main findings suggest that before 1984:Q1, the crude oil prices were leading the US GDP cycle by three quarters and Granger cause US GDP. In contrast, after 1984:Q1, the crude oil prices were lagging the US business cycle, and a reverse causality is found to run from US GDP to oil prices. The multiscale Granger causality tests globally corroborate these results.

14/01385 Hydroprocessing of heavy gas oils using FeW/SBA-15 catalysts: experimentals, optimization of metals loading, and kinetics study

Boahene, P. E. *et al. Catalysis Today*, 2013, 207, 101–111.

In this study, FeW/SBA-15 catalysts were prepared and screened for their hydrodesulfurization and hydrodenitrogenation activities using bitumen-derived heavy gas oil from Athabasca. A systematic process optimization study was conducted to investigate the optimum process conditions required to evaluate kinetic parameters for these reactions. Catalyst metal loadings were varied from 0 to 5 and 15 to 45 wt% for Fe and W, respectively; resulting in an optimum catalyst (Cat-5) with metal loadings of 3.0 and 30.0 wt% for Fe and W, respectively. Several techniques were employed to characterize the prepared catalysts and activity results have been correlated with that obtained from characterization. Hydrotreating experiments were performed in a continuous flow micro trickle-bed reactor at the temperatures, pressures and LHSVs of 633–693 K, 7.6–9.6 MPa and 0.5–2 h^{-1}, respectively, with H_2 flow rate and catalyst weight maintained constant at 50 mL/min and 1.5 g, respectively, in all cases. Three kinetic models were applied to fit experimental data obtained from HDS and HDN reaction studies evaluated within temperature range of 633–693 K. The optimum operating conditions for maximum sulfur and nitrogen conversions occurred at temperature, pressure and LHSV of 673 K, 8.8 MPa and 1 h^{-1}, respectively. Experimental data fitted with the power law model yielded reaction orders of 2.0 and 1.5 for HDS and HDN reactions, respectively; and activation energies of 129.6 and 150.6 kJ/mol, respectively. By fitting a modified power law model (multi-parameter model) to the kinetic data yielded hydrodesulfurization and hydrotreating reactions orders of 2.2 and 1.8, with respective activation energies of 126.7 and 118.8 kJ/mol.

14/01386 Hydrothermal liquefaction of *Chlorella pyrenoidosa* in sub- and supercritical ethanol with heterogeneous catalysts

Zhang, J. *et al. Bioresource Technology*, 2013, 133, 389–397.

Hydrothermal liquefaction (HTL) of low lipid content microalgae *Chlorella pyrenoidosa* with heterogeneous catalysts was processed under subcritical and supercritical conditions of ethanol (200–300 °C, 2.8–9.0 MPa, 30 min). The HTL products were separated into bio-crude, gas, solid residue and volatile components, and then characterized. The highest mass and energy recovery ratios of bio-crude on the dry basis of alga were 71.3% and 101.8%, respectively, obtained at 240 °C, while the highest higher heating value of bio-crude was 36.19 MJ/kg, obtained at 300 °C. Temperature was found to be the most dominant parameter. H_2 as a processing gas at an initial pressure of 1.03 MPa slightly improved the bio-crude yield and quality. Raney-Ni and HZSM-5 type zeolite catalysts had no significant effect on the presented HTL process. The results indicated that HTL with ethanol as the solvent was able to produce 50–70 wt% of bio-crude directly from *C. pyrenoidosa*.

14/01387 Seasonal patterns in daily prices of unleaded petrol across Australia

Valadkhani, A. *Energy Policy*, 2013, 56, 720–731.

This study addresses a very significant policy issue not previously examined at a disaggregated level for Australia by identifying on which day(s) petrol is more expensive and in which locations discount days are non-existent. After conducting a time series analysis of the day of the week effect in retail prices of unleaded petrol in 114 locations across Australia (January 2005 to April 2012), it is observed that prices mostly peak on Thursday/Friday and then decline until they hit their cyclical trough mainly on Sunday/Tuesday. However, these daily differences are only statistically significant in capital cities or large regional centres. A cross-sectional analysis of the mean prices during the period November 2007 to February 2012 shows that (a) in remote and less populous locations, where sales are presumably limited and overhead costs are high, petrol is more expensive and (b) petrol generally costs more in places which exhibit less price variability. The disaggregated and location-specific results can increase the understanding of Australia's retail petrol market and can be beneficial to motorists as well as various government and non-government organizations such as the Australian Competition and Consumer Commission, the Australian Automobile Association and FuelWatch.

14/01388 Zero emissions of CO_2 during the production of liquid fuel from coal and natural gas by combining Fischer–Tropsch synthesis with catalytic dehydrogenation

Huffman, G. P. *Fuel*, 2013, 109, 206–210.

Synthesis gas (syngas) produced by coal gasification typically has H_2/CO molar ratios in the range of 0.5–1.0. Fischer–Tropsch synthesis (FTS) of liquid fuels requires syngas with $H_2/CO \geq 2.0$. Traditionally,

this has achieved by the water–gas shift (WGS) reaction. In an earlier paper, it was shown that large reductions in CO_2 emissions can be achieved by producing the required H_2 by catalytic dehydrogenation (CDH) of the gaseous (C1–C4) products of FTS, rather than by the WGS reaction. In addition to producing pure H_2, CDH converts the C in (C1–C4) gases into multi-walled carbon nanotubes (MWCNT), a valuable by-product. The current paper builds on this concept. It is shown that zero emissions of CO_2 can be achieved by the FTS–CDH process if methane derived from natural gas is injected into the CDH reactor in appropriate amounts.

03 GASEOUS FUELS

Sources, properties, recovery, treatment

14/01389 Natural gas viscosity estimation through corresponding states based models

Heidaryan, E. *et al. Fluid Phase Equilibria*, 2013, 354, 80–88.

As natural gas viscosity is one of the most important parameters in natural gas engineering calculations, its accurate value determination plays a key role in its management. In this study, a comprehensive model is suggested for prediction of natural gas viscosity in a wide range of pressures (14.69–20,053 psia), temperatures (434–820 °R), and gas specific gravity of 0.573–1.207. The new model is applicable for gases containing heptane plus and non-hydrocarbon components. It is validated by the 3255 viscosity data from 25 different gas mixtures. The average absolute error of the model was found to be 3.03% and 5.89% in the comparison with the natural gas and gas condensate viscosity data respectively, compared to existing similar methods, its results are quite satisfactory.

14/01390 Porous media quenching behaviors of gas deflagration in the presence of obstacles

Wen, X. *et al. Experimental Thermal and Fluid Science*, 2013, 50, 37–44.

To understand the mechanism for the porous media quenching of gas deflagration in the presence of obstacles, an experimental study has been conducted, and 10 cases in a laboratory scale obstructed chamber varying in terms of the number of obstacles, porous media pore size, thickness, and material have been examined. The results show that if the premixed flame propagating away from an ignition source encounters obstacles before the flame front arrives to the porous media, the interaction between flame and obstacles will result in higher flame speed and overpressure, which may cause a failure in the operation of porous media quenching. The porous media quenching behaviour is dependent on the number of the obstacles in the flame path. Moreover, the smaller the pore size or the thicker the porous media plate, the better the flame quenching performance, but the larger the drop of the overpressure for flow-through the porous media. The material of the porous media is also found to have a significant effect on the quenching characteristics of gas deflagration. Compared to Al_2O_3 and SiC, the Al porous media shows superior flame quenching and overpressure attenuating performances. Mechanisms for the observed phenomena are discussed.

Transport, storage

14/01391 Correlation of turbulent burning velocity for syngas/air mixtures at high pressure up to 1.0 MPa

Wang, J. *et al. Experimental Thermal and Fluid Science*, 2013, 50, 90–96.

Instantaneous flame front structures of the turbulent premixed flames of syngas/air and CH_4/air mixtures were investigated using OH-PLIF technique at high pressure up to 1.0 MPa, through which the turbulent burning velocities were derived and correlated with the turbulence intensity. Results show that both syngas/air and CH_4/air mixtures, S_T/S_L increases remarkably with the increase of u'/S_L particularly in the weak turbulence region. For the syngas/air mixture, the intensity of flame front wrinkle is promoted with the increase of hydrogen fraction in the syngas due to the increased preferential diffusive-thermal instability. Compared to CH_4/air mixture, the syngas flames possess much wrinkled flame front with much smaller fine cusps structure, and with increasing u'/S_L, the rate of the increase of S_T/S_L for the syngas/air mixtures is more significant than that of CH_4/air mixtures. This demonstrates that the increase of flame front area due to turbulence wrinkling is promoted by flame intrinsic instability for syngas/air mixtures. The values of S_T/S_L for all mixtures increase with the increase of pressure because of the decrease of flame thickness which promotes the hydrodynamic instability. A general correlation of turbulent burning velocity for the syngas/air and CH_4/air mixtures was obtained in the form of $S_T/S_L \propto a[(P/P_0)(u'/S_L)]^n$.

14/01392 Geochemical modelling of CO_2–water–rock interactions in a potential storage formation of the north German sedimentary basin

Mitiku, A. B. *et al. Applied Geochemistry*, 2013, 36, 168–186.

The lower Triassic/Bunter sandstone and lower Jurassic/Rhät formations of the northern Germany sedimentary basin constitute feasible reservoirs for the storage of CO_2 from combustion of fossil fuels or industrial production processes. This study presents analyses of geochemical interactions between CO_2, formation fluid and rock of these potential reservoirs using geochemical modelling in order to assess the short- and long-term impact of CO_2 sequestration. Batch equilibrium modelling was performed first for assessing the consistency of fluid and mineralogy field data and for identifying potential secondary minerals under the influence of injected CO_2. Inclusion of reaction kinetics in the batch models allowed an observation of reaction paths and to estimate the time frame of geochemical reactions. Finally, one-dimensional equilibrium reactive transport modelling was used in order to investigate the direction of reactions under conditions of fluid flow and mass transport and to quantify feedbacks of reactions on transport processes. Results of the simulations performed show that dawsonite may act as the main CO_2 storage mineral in both formations, while the carbonates calcite and dolomite dissolve over time. Also, changes in porosity and permeability are significant in the equilibrium reactive transport simulations. The timescale of kinetically controlled reactions observed in the kinetic batch modelling, however, suggests that CO_2 mineral trapping in both formations requires very long time frames, and hence other mechanisms such as structural or solubility trapping seem to be more relevant within the injection or early post-injection phase for the studied formations.

14/01393 Nitrogen removal from natural gas using solid boron: a first-principles computational study

Sun, Q. *et al. Fuel*, 2013, 109, 575–581.

Selective separation of nitrogen (N_2) from methane (CH_4) is highly significant in natural gas purification, and it is very challenging to achieve this because of their nearly identical size (the molecular diameters of N_2 and CH_4 are 3.64 and 3.80 Å, respectively). Here the authors theoretically study the adsorption of N_2 and CH_4 on B_{12} cluster and solid boron surfaces α-B_{12} and γ-B_{28}. The results show that these electron-deficiency boron materials have higher selectivity in adsorbing and capturing N_2 than CH_4, which provides very useful information for experimentally exploiting boron materials for natural gas purification.

Economics, business, marketing, policy

14/01394 Exploring the uncertainty around potential shale gas development – a global energy system analysis based on TIAM (TIMES Integrated Assessment Model)

Gracceva, F. and Zeniewski, P. *Energy*, 2013, 57, 443–457.

This paper aims to quantitatively explore the uncertainty around the global potential of shale gas development and its possible impacts, using a multi-regional energy system model, TIMES Integrated Assessment Model (TIAM). Starting from the premise that shale gas resource size and production cost are two key preconditions for its development, this scenario analysis reveals the way these and other variables interact with the global energy system, impacting on the regional distribution of gas production, interregional gas trade, demand and prices. The analysis shows how the reciprocal effects of substitutions on both the supply and demand-side play an important role in constraining or enabling the penetration of shale gas into the energy mix. Moreover, the authors systematically demonstrate that the global potential for shale gas development is contingent on a large number of intervening variables that manifest themselves in different ways across regionally-distinct energy systems. A simple theoretical model is derived from the results of the scenario analysis. Its purpose is to simplify and explain the complex behaviour of the system, by illustrating the chain of actions and feedbacks induced by different shale gas economics, their magnitude, their relative importance, and the necessary conditions for the global potential to be realized.

Derived gaseous fuels

14/01395 A syngas network for reducing industrial carbon footprint and energy use

Roddy, D. J. *Applied Thermal Engineering*, 2013, 53, (2), 299–304.

This paper makes a case for building syngas networks as a means of contributing to the reduction of industrial carbon footprints. After exploring historic and conventional approaches to producing syngas (or synthesis gas) from fossil fuels on increasingly large scales, the paper looks at ways of producing it from renewable sources and from surplus resource (or waste) from industrial, domestic, urban and agricultural systems. The many ways of converting syngas into power, industrial heat, fuels, chemical feedstocks and chemical products are then outlined along with the associated syngas purification requirements. Some of the processes involved provide an opportunity for cost-effective capture and storage of CO_2. Pathways through this range of possibilities that enable a net reduction in energy footprint or in CO_2 emissions are identified and exemplified. Recognizing that those opportunities are likely to involve industrial facilities that are distributed spatially within a geographic area, the case for building an interconnecting syngas network is explored. Issues surrounding sizing the network, timing its growth, determining ownership and access arrangements, and planning/regulatory hurdles are found to be similar to the analogous case of building an industrial CO_2 network, with the added complication that the term 'syngas' tends to be used to cover a fairly wide range of gas compositions.

14/01396 Application of random pore model for synthesis gas production by nickel oxide reduction with methane

Rashidi, H. *et al. Energy Conversion and Management*, 2013, 74, 249–260.

Recently, there is a great interest in the non-catalytic gas–solid reactions between methane, as an environmentally friendly reducing agent, and metal oxides to yield synthesis gas and the related metal at low temperatures. In the present work, reduction of nickel oxide with methane was investigated. It has been proven that it is possible to produce metallic nickel and synthesis gas, simultaneously. The thermogravimetry measurements and instantaneous mass spectrometry analysis of the gaseous products have been performed for the $NiO + CH_4$ reaction. In addition, the complete mathematical model was developed by applying the random pore model to predict the conversion–time profiles at the temperature range of 600–750 °C. Some important parameters such as concentration dependency, external mass transfer resistance, solid structural changes, product layer resistance, and pore size distribution have been considered in this sophisticated mathematical model. In addition, the random pore model has been modified for consideration of the bulk flow effect. Results obtained from this kinetic study indicate that the model performs well in predicting the experimental data. However by neglecting the bulk flow effect, there are lower predicted rate constants for this reaction. The analysis of the gaseous products showed that the synthesis gas could be produced with a H_2/CO ratio near to two.

14/01397 Catalytic behavior of Ni-modified perovskite and doped ceria composite catalyst for the conversion of odorized propane to syngas

Lo Faro, M. *et al. Fuel Processing Technology*, 2013, 113, 28–33.

The catalytic activity of a Ni-modified perovskite (LSFCO)–ceria-doped gadolinia composite catalyst in the presence of odorized propane has been studied in order to assess this material as catalyst for a fuel processor in solid oxide fuel cells (SOFCs). At first, the study involved the investigation of the catalytic activity in the presence of propane in different reaction conditions and temperatures. Once established the best reaction conditions, the catalytic stability in an endurance test, and subsequently the effect on the catalytic performance of adding different amounts of H_2S, has been explored. The autothermal reforming (ATR) at 800 °C has provided the highest performance (99% C_3H_8 conversion, 67% H_2 and 17% CO yields). The upper limit of H_2S content in propane for which the performance of such catalyst is still acceptable in terms of propane conversion and syngas yield is 80 ppm. Accordingly, the level of sulfur contaminants tolerated by this catalyst is much higher than that of conventional Ni-based catalyst for similar conversion and syngas yield.

14/01398 Catalytic steam gasification of pig compost for hydrogen-rich gas production in a fixed bed reactor

Wang, J. *et al. Bioresource Technology*, 2013, 133, 127–133.

The catalytic steam gasification of pig compost (PC) for hydrogen-rich gas production was experimentally investigated in a fixed bed reactor using the developed NiO on modified dolomite (NiO/MD) catalyst. A series of experiments have been performed to explore the effects of catalyst, catalytic temperature, steam to PC ratio and PC particle size on the gas quality and yield. The results indicate that the NiO/MD catalyst could significantly eliminate the tar in the gas production and increase the hydrogen yield, and the catalyst lives a long lifetime in the PC steam gasification. Moreover, the higher catalytic temperature and smaller PC particle size can contribute to more hydrogen production and gas yield. Meanwhile, the optimal ratio of steam to PC (S/P) is found to be 1.24.

14/01399 Fischer–Tropsch synthesis: Mössbauer investigation of iron containing catalysts for hydrogenation of carbon dioxide

Gnanamani, M. K. *et al. Catalysis Today*, 2013, 207, 50–56.

CO_2 hydrogenation was investigated with a doubly promoted (Cu, K) silica containing iron catalyst. Hägg carbide (χ-Fe_5C_2) is the dominant phase obtained under CO activation conditions at 543 K and 0.1 MPa and it was stable under Fischer–Tropsch synthesis (FTS) conditions typical for coal- or biomass-derived syngas using a H_2/CO ratio of 1 : 1 for at least ~100 h TOS. An Fe-phase change occurs (χ-$Fe_5C_2 \rightarrow Fe_3O_4$) after switching from $H_2 : CO : N_2$ (1 : 1 : 2) to $H_2 : CO_2$ (3 : 1). The distribution of hydrocarbon products changes significantly after switching to $H_2 : CO_2$ (3 : 1), but then it slowly transformed to normal FTS products, albeit with over three times higher methane selectivity compared to FTS using $H_2 : CO : N_2$ (1 : 1 : 2). A correlation was obtained between the rate of FTS and the percentage of Fe carbide indicating that iron carbide is the active phase for CO_2-based FTS. Irrespective of conditions (i.e. either $H_2 : CO : N_2 = 1 : 1 : 2$ or $H_2 : CO_2 = 3 : 1$) and the Fe phase, the methane selectivity appears to primarily depend on the H_2/CO ratio.

14/01400 Inhibition of carbon formation during steam reforming of methane over ethyldisulfide-impregnated metallic nickel catalysts

Priya, K. S. *et al. Catalysis Today*, 2013, 207, 21–27.

This paper describes the surface modification of unsupported micrometric nickel powder with ethyldisulfide and its use as a catalyst in steam reforming of methane (SRM). It reports on catalytic activity and inhibition of carbon formation due to unsupported Ni catalyst alterations with varying ethyldisulfide molar ratios. Methane conversion was investigated by mass spectrometry under time-on-stream conditions during SRM reactions at a temperature = 700 °C for 12 h at methane/steam molar ratio = 1 : 2 and gas hourly space velocity = 19,600 ml g^{-1} h^{-1}; selectivity toward hydrogen production and CO and CO_2 formation was calculated. The nature and relative quantities of carbon species formed on the surface of spent catalysts were studied by X-ray photoelectron spectroscopy analysis. A preliminary mechanistic explanation regarding the inhibition of C formation over the used modified catalysts is provided.

14/01401 Pressurised gasification of wet ethanol fermentation residue for synthesis gas production

Koido, K. *et al. Bioresource Technology*, 2013, 131, 341–348.

Pressurized steam gasification of wet biomass in a fixed-bed downdraft gasifier was implemented to identify reaction conditions yielding the highest synthesis gas concentration and efficiency, and to examine the generation of sulfur compounds. The gasification of lignin-rich fermentation residue derived from a bench-plant for bioethanol production from woody biomass was investigated at $p = 0.99$ MPa and $T = 750$–900 °C for steam to biomass ratios (S/B) of 3.4–17 and equivalence ratios (ψ) of 3.3–∞. The results showed that the highest concentration of around 70 mol% was obtained at $T \geq 850$ °C, $\psi = 13$ and $S/B = 3.4$, the highest efficiency of 0.26 was obtained at $T = 900$ °C, $\psi = 3.3$ and $S/B = 3.4$, and sulfur compounds were H_2S and COS. For the production of BTL synthesis gas, pressurized gasification has the potential to convert the wet residue below 77.3 wt% moisture contents.

14/01402 Syngas from steam gasification of polyethylene in a conical spouted bed reactor

Erkiaga, A. *et al. Fuel*, 2013, 109, 461–469.

The steam gasification of high-density polyethylene in continuous mode has been carried out in a conical spouted bed reactor. The effect of temperature (in the 800–900 °C range) and steam/plastic mass ratio (between 0 and 2) on the distribution of products (gas and tar) and their composition has been studied. In order to reduce tar formation, two catalysts have been used *in situ*, namely, olivine and γ-Al_2O_3. The spouted bed reactor has an excellent performance between 850 and 900 °C, and an increase in the steam/plastic ratio from 1 to 2 only improves slightly both carbon conversion efficiency (to 93.6% with steam/plastic ratio = 2) and hydrogen concentration (61.6%). The use of olivine and γ-Al_2O_3 instead of sand gives way to a moderate reduction in the tar formation, whose yield is 4.8% with olivine. The syngas obtained has a H_2/CO ratio of 2.2, with a low tar content whose composition (monoaromatics, mainly benzene) augurs well for the use of the syngas in dimethyl ether synthesis.

14/01403 Syngas production by CO_2/O_2 gasification of aquatic biomass

Hanaoka, T. *et al. Fuel Processing Technology*, 2013, 116, 9–15.

In the gasification of an aquatic biomass with $He/CO_2/O_2$, the effects of the concentration of CO_2 and O_2 in the gasifying agent and the feeding rate on the gasification behaviour were investigated using a downdraft fixed-bed gasifier at 900 °C. Using CO_2/O_2 as the gasifying agent led to an increase in the conversion to gas and the syngas ($CO + H_2$) content because the gasification of char with CO_2 ($C + CO_2 \rightarrow 2CO$) and the decomposition of tarry compounds were promoted. Increasing CO_2 content led to the increase in the conversion to gas and CO content and the decrease in the H_2 content. With increasing O_2 content, contents of CO and H_2 increased while the conversions to gas remained almost constant. Especially with $CO_2/O_2 = 45/55$ vol.%, the conversion to gas was 94.0 C-mol% and the syngas content exhibited a maximum value of 69.7 vol.%. As the feeding rate was decreased, contents of CO and H_2 decreased while the conversion to gas remained almost constant. The nitrogen atoms in the feedstock were mainly converted to form N_2. H_2S and COS were the main sulfurous gases. The sulfur content in the char was much higher than that in the feedstock.

14/01404 Woody waste air gasification in fluidized bed with Ca- and Mg-modified bed materials and additives

Kuo, J.-H. *et al. Applied Thermal Engineering*, 2013, 53, (1), 42–48.

This study focuses on the promotion of biomass gasification for hydrogen production in a fluidized bed reactor with the bed additives zeolite, CaO, and Ca- and Mg-based silica sands. The results show that zeolite has higher capacity for enhancing hydrogen promotion abilities than CaO with the amount was 200 g in tests. Regarding the Ca- and Mg-based silica sands, Ca/SiO_2 decreases the CO_2 selectivity and Mg/SiO_2 enhances the H_2 selectivity owing to CO_2 adsorption via the formation of CaO and the promotion of the water gas shift reaction, respectively. The optimal concentration of Mg-based bed materials corresponds to a Mg concentration of 0.5 wt%. The additives play important roles in increasing the reaction rate, enhancing the biomass gasification, and promoting carbon transformation.

LNG

14/01405 A novel NGL (natural gas liquid) recovery process based on self-heat recuperation

Van Duc Long, N. and Lee, M. *Energy*, 2013, 57, 663–670.

This study examined an innovative self-heat-recuperation technology that circulates latent and sensible heat in the thermal process and applied it to the natural gas liquid recovery process. A column grand composite curve was used to assess the thermodynamic feasibility of implementing the heat pump system and self-heat-recuperation technology into a conventional distillation column. The proposed distillation based on self-heat recuperation reduced the energy consumption dramatically by compressing the effluent stream, whose temperature was increased to provide the minimum temperature difference for the heat exchanger, and circulating the stream heat in the process. According to a simulation of the proposed sequence, up to 73.43 and 83.48% of the condenser and reboiler energy, respectively, were saved compared to a conventional column. This study also proposes heat integration to improve the performance of self-heat recuperation. The results showed that the modified sequence saves up 64.35, 100.00 and 31.60% of the condenser energy requirements, reboiler energy requirements and operating cost, respectively, compared to a classical heat pump system, and 90.24, 100.00, and 67.19%, respectively, compared to a conventional column. The use of these sequences to retrofit a distillation column to save energy was also considered.

14/01406 Experimental research on the effects of fluid and heater on thermal stratification of liquefied gas

Shi, J. *et al. Experimental Thermal and Fluid Science*, 2013, 50, 29–36.

The thermal stratification of liquefied gas influences the equipment safety. To find the factors and principles governing the thermal stratification, a device was set up to simulate the thermal response of a liquefied gas tank. A small steel vessel was used to simulate the tank, and two working fluids were used: water and R22. The heating region and liquid level were precisely adjusted in the tests to simulate different accident conditions. The experimental results showed saturation pressure of the working fluid affected the thermal stratification when the liquid wall was heated solely. For the case the liquid and vapour wall were heated together, evident thermal stratifications formed both in R22 and water tests. The degree and duration of thermal stratification are affected by the intensity of heat loading on the surface liquid. It is concluded that nucleate boiling in the lower liquid has great power to eliminate the thermal stratification. When the nucleate boiling is suppressed by hydrostatic pressure or saturation pressure of the warm surface liquid, the thermal stratification can form and maintain by natural convection. The stratifying process can be explained by a natural convection model.

14/01407 Improving sustainability of maritime transport through utilization of liquefied natural gas (LNG) for propulsion

Burel, F. *et al. Energy*, 2013, 57, 412–420.

Today, most merchant vessels use heavy fuel oils for ship propulsion. These fuels are cost effective but they produce significant amounts of noxious emissions. In order to comply with International Maritime Organization rules, liquefied natural gas (LNG) is becoming an interesting option for merchant ships. The aim of the research presented in this paper is to analyse the economic upturn that can result from the use of LNG as fuel for merchant ships and to assess the effects of its utilization in terms of environmental impact. In the first part of the study, a statistical analysis of maritime traffic is carried out in order to identify which merchant ship types could most benefit from using LNG as fuel for ship propulsion. Traffic data of world ships related to the months of May 2008, 2009 and 2010 are analysed. Roll-on/roll-off vessels and tanker ships spend most of their sailing time in emission control areas consequently appear to be the best candidates for LNG use. In particular, the use of LNG is most profitable for tanker ships in the range of 10,000–60,000 DWT (deadweight). In the second part of the study, operational costs and pollutant emission reduction, following LNG implementation, are calculated for a 33,000 DWT tanker ship. Results show that LNG leads to a reduction of 35% of operational costs and 25% of CO_2 emissions. The possibility of improving energy efficiency on board is analysed considering that combustion gases, produced by LNG, are cleaner, thus simplifying the introduction of exhaust gas heat recovery. Two options are considered: simple heat recovery and heat recovery to drive a turbine. The results show that it is possible to achieve a reduction in fuel consumption of up to 15%.

Hydrogen generation and storage

14/01408 An energy self-sufficient public building using integrated renewable sources and hydrogen storage

Marino, C. *et al. Energy*, 2013, 57, 95–105.

The control of the use of fossil fuels, major cause of greenhouse gas emissions and climate changes, in present days represents one of Governments' main challenges; particularly, a significant energy consumption is observed in buildings and might be significantly reduced through sustainable design, increased energy efficiency and use of renewable sources. At the moment, the widespread use of renewable energy in buildings is limited by its intrinsic discontinuity: consequently integration of plants with energy storage systems could represent an efficient solution to the problem. Within this frame, hydrogen has shown to be particularly fit in order to be used as an energetic carrier. This study presents an energetic, economic and environmental analysis of two different configurations of a self-sufficient system for energy production from renewable sources in buildings. In particular, in the first configuration energy production is carried out by means of photovoltaic systems, whereas in the second one a combination of photovoltaic panels and wind generators is used. In both configurations, hydrogen is used as an energy carrier, in order to store energy, and fuel cells guarantee its energetic reconversion. The analysis shows that, although dimensioned as a stand-alone configuration, the system can today be realized only taking advantage from the incentivizing fares applied to grid-connected systems, that are likely to be suspended in the next future. In such case, it represents an interesting investment, with capital returns in about 15 years. Regarding economic sustainability, in fact, the analysis shows that the cost of the energy unit stored in hydrogen volumes, due to the not very high efficiency of the process, presently results greater than that of directly used one. Moreover, also the starting fund of the system proves to be very high, showing an additional cost with respect to systems lacking of energy storage equal to about 50%. From the above, it can be deduced that, in the aim to obtain a quick, effective penetration of hydrogen into the market, it is at the moment indispensable to enact incentivizing policies, attributing to hydrogen production fares able to cover the additional costs due to its production, storage and reconversion.

14/01409 Bio-electrolytic conversion of acidogenic effluents to biohydrogen: an integration strategy for higher substrate conversion and product recovery

Babu, M. L. *et al. Bioresource Technology*, 2013, 133, 322–331.

Feasibility of integrating microbial electrolysis cell (MEC) process with dark-fermentation process for additional hydrogen recovery as well as substrate degradation was demonstrated in the present study. MEC was employed in order to utilize the residual organic fraction present in the acidogenic effluents of dark fermentation process as substrate for hydrogen production with input of small electric current. MEC was operated at volatile fatty acids (VFA) concentration of 3000 mg/l under different poised potentials (0.2, 0.5, 0.6, 0.8 and 1.0 V) using anaerobic consortia as biocatalyst. Maximum hydrogen production rate (HPR), cumulative hydrogen production (CHP) (0.53 mmol/h and 3.6 mmol), dehydrogenase activity (1.65 μg/ml) and VFA utilization (49.8%) was recorded at 0.6 V. Bio-electrochemical behaviour of mixed consortia was evaluated using cyclic voltammetry and by Tafel slope analysis. Microbial diversity analysis using denaturing gradient gel electrophoresis confirmed the presence of gammaproteobacteria (50%), bacilli (25%) and clostridia (25%).

14/01410 Design of a hydrogen production process for power generation based on a Ca-Cu chemical loop

Martínez, I. *et al. Energy Procedia*, 2013, 37, 626–634.

This work proposes the integration into a natural gas combined cycle (NGCC) of a novel H_2 production process based on a double chemical Ca–Cu loop. This hydrogen-production process is based on the sorption enhanced reforming process including a CaO-based solid as a high-temperature CO_2 sorbent. The addition of a second CuO/Cu loop provides the energy required to carry out the sorbent regeneration. The coupling between this process and a combined cycle is discussed in the paper, and an efficiency assessment of the whole plant is determined. A total of 9.5 percentage points of efficiency penalty has resulted from the integration proposed, which is in the range of those penalties reported for autothermal reforming, partial oxidation or sorption-enhanced water gas shift integrated with a combined cycle. Ca–Cu looping performance could be improved if fewer exigent conditions were chosen, which adds to the inherent advantages of cheaper reactor design, feasible solid materials and fewer process units, making the Ca–Cu looping process emerge as a potential pre-combustion CO_2 capture technology.

14/01411 Efficiency of the sulfur–iodine thermochemical water splitting process for hydrogen production based on ADS (accelerator driven system)

García, L. *et al. Energy*, 2013, 57, 469–477.

The current hydrogen production is based on fossil fuels; they have a huge contribution to the atmosphere's pollution. Thermochemical water splitting cycles don not present this issue as the required process heat is obtained from nuclear energy and therefore, the environmental impact is smaller than using conventional fuels. Solar hydrogen production could be also used because of its lower environmental impact. One of the most promising approaches to produce large quantities of hydrogen in an efficient way using nuclear energy is the sulfur–iodine thermochemical water splitting cycle. The nuclear source proposed in this paper is a pebble bed gas cooled transmutation facility. Pebble bed very high temperature advanced systems have great perspectives to assume the future nuclear energy. Software based on chemical process simulation can be used to simulate the thermochemical water splitting sulfur–iodine cycle for hydrogen production. In this paper, a model for analysing the sulfur–iodine process sensibility respect to the thermodynamics parameters: temperature, pressure and mass flow is developed. Efficiency is also calculated and the influence of different parameters on this value. The behaviour of the proposed model for different values of initial reactant's flow, is analysed.

14/01412 Magnesium–carbon hydrogen storage hybrid materials produced by reactive ball milling in hydrogen

Lototskyy, M. *et al. Carbon*, 2013, 57, 146–160.

Time-resolved studies uncovered kinetics and mechanism of Mg–hydrogen interactions during high energy reactive ball milling in hydrogen (HRBM) in presence of various types of carbon, including graphite (G), activated carbon (AC), multi-wall carbon nanotubes (MWCNT), expandable (EG) and thermally expanded (TEG) graphite. Introduction of carbon significantly changes the hydrogenation behaviour, which becomes strongly dependent on the nature and amount of carbon additive. For the materials containing 1 wt% AC or TEG, and 5 wt% MWCNT, the hydrogenation becomes superior to that for the individual magnesium and finishes within 1 h. Analysis of the data indicates that carbon acts as a carrier of the 'activated' hydrogen by a mechanism of spill-over. For Mg–G the hydrogenation starts from an incubation period and proceeds slower. An increase in the content of EG and TEG above 1 wt% results in the deterioration of the hydrogenation kinetics. The effect of carbon additives has roots in their destruction during the HRBM to form graphene layers encapsulating the MgH_2 nanoparticles and preventing the grain growth. This results in an increase of absorption–desorption cycle stability and a decrease of the MgH_2 crystallite size in the re-hydrogenated Mg–C hybrid materials (40–125 nm) as compared to Mg alone (180 nm).

14/01413 Production of hydrogen by steam reforming of methane over alumina supported nano-NiO/SiO_2 catalyst

Bej, B. *et al. Catalysis Today*, 2013, 207, 28–35.

Steam reforming of methane (SRM) was carried out over alumina supported nano NiO catalyst in silica synthesized using sol–gel method. The crystallite size of NiO in NiO–SiO_2 catalysts was found to vary with the calcination temperature and the extent of Ni loading in the catalyst. The NiO crystallite size was found to be 9–15 nm in the Ni loading range of 5–15% and calcinations temperature range of 350–500 °C studied. Catalyst containing 10% Ni was found to be the best one for steam reforming reaction in terms of methane conversion. The catalyst was found to be very active and stable in the temperature range of 500–700 °C. The most favourable reaction condition was established at a temperature of 700 °C, steam to methane molar ratio of 3.5 and a space–time of 11.31 kg cat h/kmol of inlet methane. At this optimum condition, the conversion of methane was 95.7% and the yield of hydrogen was about 3.8 moles of hydrogen per mole of methane reacted.

14/01414 Steam reforming of acetic acid for hydrogen production over bifunctional Ni–Co catalysts

Pant, K. K. *et al. Catalysis Today*, 2013, 207, 36–43.

Bio-oil derived from biomass can be used to produce hydrogen, which is important for the future global economy. In this study, steam reforming of acetic acid was conducted in a fixed bed reactor with different supported metal catalysts in a temperature range of 500–750 °C. In this study Ni–Co, Ni–Co/CeO_2/ZrO_2 and lanthanum oxide promoted Ni/La_2O_3/Al_2O_3 catalysts were prepared either by wet impregnation or by co-precipitation method and characterized by XRD, SEM–EDX, TG-DTA, BET and TEM analysis. It was found that bimetallic and without support catalyst Ni–Co (0.25 : 1) had higher activity and H_2 yield compared with Ni–Co/CeO_2/ZrO_2 and 17% Ni/La_2O_3/Al_2O_3 catalysts. The effects of reaction temperature, space time (W/F_{A0}), acetic acid feed concentration and time-on-stream were studied in detail over Ni–Co catalyst.

14/01415 Synthesis and characterization of magnesium–carbon compounds for hydrogen storage

Kubota, A. *et al. Carbon*, 2013, 56, 50–55.

Magnesium (Mg) and carbon (C) compounds were synthesized by ball-milling a mixture of Mg and different graphites with different crystallinities. The materials were characterized by X-ray diffraction, X-ray absorption spectroscopy, and X-ray total scattering techniques. Hydrogen storage properties were also investigated. In the case of the material using low-crystalline graphite, a Mg and C compound was formed as main phase, and its chemical bonding state was similar to that of magnesium carbide (Mg_2C_3). The hydrogen absorption reaction of the Mg–C compound occurred at around 400 °C under 3 MPa of hydrogen pressure to form magnesium hydride (MgH_2) and the C–H bonds in the carbon material. The hydrogenated Mg–C material desorbed about 3.7 mass% of hydrogen below 420 °C with two processes, which were the decomposition of MgH_2 and the subsequent reaction of the generated Mg and the C–H bonds. From the results, it is concluded that the Mg–C compound absorb and desorb about 3.7 mass% of hydrogen below 420 °C.

04 BY-PRODUCTS RELATED TO FUELS

14/01416 Changes in trace element contents in ashes of oil shale fueled PF and CFB boilers during operation

Reinik, J. *et al. Fuel Processing Technology*, 2013, 115, 174–181.

Two oil shale combustion technologies, pulverized firing (PF) and circulated fluidized bed (CFB) were compared with respect to partitioning of selected elements (Ba, Cd, Co, Cr, Cu, Hg, Mn, Mo, Ni, Pb, Rb, Sb, Sn, Sr, Th, Tl, U, V, and Zn) in the ashes along the flue gas ducts. The ash samples were characterized by high-resolution ICP-MS. The average contents of toxic heavy metals in fly ash samples from the CFB boiler are lower compared to the PF boiler. Main differences in trace element contents between combustion technologies were as follows: Cd content in the fly ash samples of PF boiler was up to 0.9 mg/kg while in CFB boiler it remained below 0.1 mg/kg in all analysed ash samples; Hg was observed in the ashes of electrostatic precipitator (ESP) of CFB boiler while in the PF boiler it was close to or below detection limit. In the PF boiler content of Sn was detected only in the

ashes of ESPs, while in CFB boiler it was evenly distributed between bottom and fly ash samples. Highest content among heavy metals in ash samples was observed for Pb in the last field of ESP of the PF boiler (142 mg/kg).

14/01417 Electrospun carbon nanofibers from polyacrylonitrile blended with activated or graphitized carbonaceous materials for improving anodic bioelectrocatalysis

Patil, S. A. *et al. Bioresource Technology*, 2013, 132, 121–126.

The electrospun carbon nanofibres obtained from polyacrylonitrile (PAN) and PAN blends with either activated carbon (PAN-AC) or graphite (PAN-GR) were tested as anodes using *Shewanella oneidensis* MR-1. Extensive physico-chemical and electrochemical characterization confirmed their formation, their fibrous and porous nature, and their suitability as electrodes. N_2 adsorption measurements revealed high specific surface area (229.8, 415.8 and 485.2 $m^2 g^{-1}$) and porosity (0.142, 0.202 and 0.239 $cm^3 g^{-1}$) for PAN, PAN-AC and PAN-GR, respectively. The chronoamperometric measurements showed a considerable decrease in start-up time and more than a 10-fold increase in the generation of current with these electrodes (115, 139 and 155 $\mu A\,cm^{-2}$ for PAN, PAN-AC and PAN-GR, respectively) compared to the graphite electrode (11.5 $\mu A\,cm^{-2}$). These results indicate that the bioelectrocatalysis benefits from the blending of PAN with activated or graphitized carbonaceous materials, presumably due to the increased specific surface area, total pore volume and modification of the carbon microstructure.

14/01418 Fly ash supported scandium triflate as an active recyclable solid acid catalyst for Friedel–Crafts acylation reaction

Rani, A. *et al. Fuel Processing Technology*, 2013, 116, 366–373.

Coal-generated fly ash is converted into an efficient solid Lewis acid catalyst by loading scandium triflate on thermally and chemically activated fly ash. The activation of fly ash increased the surface silanol groups responsible for loading of scandium triflate species on fly ash surface. The physicochemical properties of prepared fly ash supported scandium triflate (FST) catalyst were examined by XRD, FTIR, TEM and TGA analysis. The proposed model structure of FST shows that the triflate species withdraws the electron density from the scandium resulting in generating electron deficient Lewis acid sites on fly ash surface as confirmed by NH_3 adsorbed FT-IR spectrum of FST catalyst. The catalyst showed higher activity for solvent free single pot Friedel–Crafts acylation of 2-methoxynaphthalene using acetic anhydride as an acylating agent achieving conversion up to 84% and selectivity of the desired product, 2-acetyl-6-methoxynaphthalene (6-AMN) up to 73%. 6-AMN is a precursor for anti-inflammatory drug, (S)-(+)-6-methoxy-α-methyl-2-naphthaleneacetic acid, known as Naproxen. The stability of the catalyst was confirmed by hot filtration test. The catalyst could be easily regenerated and reused giving similar conversion up to three reaction cycles under similar experimental conditions. The work reports an alternative pathway for utilization of waste fly ash by using it in developing novel and cost effective, recyclable catalyst system for industrially important acylation reactions.

14/01419 Sources and transport of black carbon at the California–Mexico border

Shores, C. A. *et al. Atmospheric Environment*, 2013, 70, 490–499.

At international border areas that suffer from poor air quality, assessment of pollutant sources and transport across the border is important for designing effective air quality management strategies. As part of the Cal–Mex 2010 field campaign at the USA–Mexico border in San Diego and Tijuana, the authors measured black carbon (BC) concentrations at three locations in Mexico and one in the USA. The measurements were intended to support the following objectives: to characterize the spatial and temporal variability in BC, to estimate the BC emission inventory, to identify potential source areas of BC emissions, and to assess the cross-border transport of BC. Concentrations at Parque Morelos, the campaign's supersite, averaged 2.2 $\mu g\,m^{-3}$ and reached a maximum value of 55.9 $\mu g\,m^{-3}$ (1-min average). Sharp, regularly occurring peaks around midnight were suggestive of clandestine industrial activity. BC concentrations were more than two times higher, on average, in Tijuana compared to San Diego. BC and carbon monoxide (CO) were strongly correlated at the three sites in Mexico. The $\Delta BC/\Delta CO$ ratio of $5.6 \pm 0.5\,\mu g\,m^{-3}\,ppm^{-1}$ in Tijuana, or $4.7 \pm 0.5\,\mu g\,m^{-3}\,ppm^{-1}$ when adjusted for seasonal temperature effects to represent an annual average, was comparable to that in other urban areas. Tijuana's emissions of BC were estimated to be 230–890 tonnes per year, 6–23% of those estimated for San Diego. Large uncertainties in this estimate stem mainly from uncertainties in the CO emission inventory, and the lower end of the estimate is more likely to be accurate. Patterns in concentrations and winds suggest that BC in Tijuana was usually of local origin. Under typical summertime conditions such as those observed during the study, transport from Tijuana into the USA was common, crossing the border in a northeasterly direction, sometimes as far east as Imperial County at the eastern edge of California.

14/01420 Synthesis and characterization of activated carbon from natural asphaltites

Tsyntsarski, B. *et al. Fuel Processing Technology*, 2013, 116, 346–349.

A possibility for utilization of natural asphaltites, based on production of carbon adsorbents, was investigated. Various combinations of physical and chemical activation as well as demineralization procedures were used to obtain final products from natural asphaltites. Carbon adsorbents with developed pore structure and with alkaline character of the surface, as well as tar and gas products, were obtained by water vapour pyrolysis of natural asphaltites. The obtained carbon adsorbents show good adsorption properties; however, this performance is somewhat limited, probably due to their high mineral and sulfur content. It was established that hydropyrolysis is not appropriate method for production of carbon adsorbents on the base of asphaltites from Sirnak deposit due to the material coking. However, a two-stage process, including carbonization and subsequent activation, is appropriate for obtaining of carbon adsorbent with developed pore structure from Sirnak asphaltites. At the same time, hydropyrolysis is suitable for obtaining of activated carbon using asphaltites from Silopi deposit. Different oxygen groups were detected on the activated carbon surface, and their effect on surface properties of the samples was discussed.

14/01421 The use of coal combustion fly ash as a soil amendment in agricultural lands (with comments on its potential to improve food security and sequester carbon)

Ukwattage, N. L. *et al. Fuel*, 2013, 109, 400–408.

The growing dependence on coal-fired electricity generation has resulted accumulation of massive quantities of coal combustion by-products such as fly ash and bottom ash which are regarded as problematic solid wastes all over the world. Being used beneficially in very less quantities, each year large amount of fly ash is disposed to arable lands which lead to degradation and contamination of land and ground water. However fly ash is identified as a useful soil ameliorant with its properties pertinent to the enhancement of soil fertility and productivity. Fly ash has the potential to improve soil physical, chemical and biological properties and is a source of readily available plant macro and micro-nutrients. Especially for countries whose soils show inherent structural and nutritional limitations for cropping and that need expensive and intensive management, fly ash creates a possible solution to improve crop yields and enhance food security. At the same time the soil added fly ash can involve in terrestrial carbon sequestration by enhancing the microclimate of the soils to facilitate organic matter humification to yield stable forms of soil carbon. This paper reviews the studies of fly ash as a soil amendment in order to present a comprehensive view of the possibility of using fly ash in agricultural lands to improve soil productivity while harvesting possible carbon sequestration benefits. Some identified adverse effects of fly ash addition that can hinder the crop growth in amended soils especially in long-term applications have limited its potential use in cultivable lands. However more research work on existing gaps in knowledge to be filled (especially regarding the appropriate application rate and possible environmental contamination) may help to derive the maximum advantages of fly ash in terms soil improvement and waste disposal. The paper, in particularly examines the potential use of this plentiful solid waste material on soil amendment in Australian agricultural soils.

05 NUCLEAR FUELS

Scientific, technical

14/01422 Analysis for impact of seismic capacity uncertainty on system reliability

Yu, Y. *et al. Energy Procedia*, 2013, 39, 183–192.

It is important for nuclear power plant safety whether the safety system can work well or not in seismic conditions. Seismic capacity data are important parameters to describe the component reliability, based on which the high confidence, low probability of failure for components can be obtained by seismic margin evaluation. However, other than median ground acceleration capacity, the aleatory and epistemic uncertainties are also key factors for component reliability, so the seismic hazard curve is one of the important affecting factors and should be taken into account in the system reliability analysis. In this paper, passive residual heat removal system in AP1000 is calculated as

an example, fault tree (FT) method is used to analyse the system reliability at different ground acceleration levels, the contribution to the system failure of components having different uncertainty parameters are given. Monte Carlo (MC) simulation is used to evaluate the system reliability in a seismic situation based on different seismic hazard curves, the effect of seismic hazard curves and seismic capacity uncertainty are put forward.

14/01423 Bond graphs for spatial kinetics analysis of nuclear reactors

Sosnovsky, E. and Forget, B. *Annals of Nuclear Energy*, 2013, 56, 208–226.

This work proposes a simple and effective approach to modelling nuclear reactor multiphysics problems using bond graphs. The bond graph formalism is a technique for modelling engineering systems as combinations of connected elements. After the bond graph representation of a multiphysics system is constructed, it can be automatically converted into a state derivative vector and integrated. Bond graphs are a flexible way of presenting coupled physics problems by automating the computer science aspects of modelling and lettings the modellers focus on the physics. Additionally, the representation of a multiport resistive element is presented, which is necessary for coupling more than two types of physics. Bond graph representations of two-dimensional multigroup neutron diffusion, delayed neutrons and thermal feedback were presented and tested using an LRA BWR control blade drop benchmark problem with a coarse mesh. The code demonstrated third-order convergence in time, a very desirable property of fully coupled time integrators.

14/01424 Evaluation of irradiation facility options for fusion materials research and development

Zinkle, S. J. and Möslang, A. *Fusion Engineering and Design*, 2013, 88, (6–8), 472–482.

Successful development of fusion energy will require the design of high-performance structural materials that exhibit dimensional stability and good resistance to fusion neutron degradation of mechanical and physical properties. The high levels of gaseous (H, He) transmutation products associated with deuterium–tritium (D–T) fusion neutron transmutation reactions, along with displacement damage dose requirements up to 50–200 displacements per atom (dpa) for a fusion demonstration reactor (DEMO), pose an extraordinary challenge. One or more intense neutron source(s) are needed to address two complementary missions: (1) scientific investigations of radiation degradation phenomena and microstructural evolution under fusion-relevant irradiation conditions (to provide the foundation for designing improved radiation resistant materials), and (2) engineering database development for design and licensing of next-step fusion energy machines such as a fusion DEMO. A wide variety of irradiation facilities have been proposed to investigate materials science phenomena and to test and qualify materials for a DEMO reactor. Some of the key technical considerations for selecting the most appropriate fusion materials irradiation source are summarized. Currently available and proposed facilities include fission reactors (including isotopic and spectral tailoring techniques to modify the rate of H and He production per dpa), dual- and triple-ion accelerator irradiation facilities that enable greatly accelerated irradiation studies with fusion-relevant H and He production rates per dpa within microscopic volumes, D–Li stripping reaction and spallation neutron sources, and plasma-based sources. The advantages and limitations of the main proposed fusion materials irradiation facility options are reviewed. Evaluation parameters include irradiation volume, potential for performing accelerated irradiation studies, capital and operating costs, similarity of neutron irradiation spectrum to fusion reactor conditions, temperature and irradiation flux stability/control, ability to perform multiple-effect tests (e.g. irradiation in the presence of a flowing coolant, or in the presence of complex applied stress fields), and technical maturity/risk of the concept. Ultimately, it is anticipated that heavy utilization of ion beam and fission neutron irradiation facilities along with sophisticated materials models, in addition to a dedicated fusion-relevant neutron irradiation facility, will be necessary to provide a comprehensive and cost-effective understanding of anticipated materials evolution in a fusion DEMO and to therefore provide a timely and robust materials database.

14/01425 How critical is turbulence modeling in gas distribution simulations of large-scale complex nuclear reactor containment?

Xiao, J. and Travis, J. R. *Annals of Nuclear Energy*, 2013, 56, 227–242.

Uncontrolled hydrogen combustion can occur in the nuclear reactor containment during a severe accident. The energetic hydrogen combustion may threaten the integrity of the containment and lead to radioactive material being released into the environment. In order to mitigate the risk of hydrogen combustion, the first step is to understand how the burnable hydrogen cloud develops in the containment. Turbulence modelling is one of the key elements in simulations of the physical phenomena that occur in containment. However, when a turbulence model is used, the computational time is increased in computational fluid dynamics (CFD) simulations of large-scale reactor containment primarily due to the additional turbulent transport equations and the small time step controlled by the explicitly-treated turbulent diffusion in GASFLOW code. The purpose of this paper is to investigate how critical turbulence modelling is in the simulation of hydrogen/steam distribution in a large-scale, complex reactor containment. In other words, is it acceptable to neglect the turbulent viscosity in the momentum diffusion term in such a large-scale engineering simulation to save computational time? The effect of turbulence models on the gas distribution in the MISTRA 2009 campaign was investigated using the CFD code, GASFLOW. The calculation results improved locally in the region near the jet source when turbulence models were used. For most of the space in the MISTRA facility, which is located away from the source, it seems that the turbulent diffusion was over-predicted by the turbulence models, and better agreements with the experimental data were obtained by simply using molecular viscosity. These results indicate that with turbulence models, more computational time is required, and the improved calculation results are local and limited. It appears that the predictions are reasonably good when only molecular viscosity is considered in the diffusion terms. Due to the limited computational resources, the trade-offs between computational effort and accuracy must be investigated, particularly in large-scale engineering applications.

14/01426 Internal inspection of reinforced concrete for nuclear structures using shear wave tomography

Scott, D. B. *Energy Conversion and Management*, 2013, 74, 582–586.

Reinforced concrete is important for nuclear-related structures. Therefore, the integrity of structural members consisting of reinforced concrete is germane to the safe operation and longevity of these facilities. Many issues that reduce the likelihood of safe operation and longevity are not visible on the surface of reinforced concrete material. Therefore, an investigation of reinforced concrete material should include techniques which will allow peering into the concrete member and determining its internal state. The performance of non-destructive evaluations is pursuant to this goal. Some of the categories of non-destructive evaluations are electrochemical, magnetism, ground penetrating radar, and ultrasonic testing. A specific ultrasonic testing technique, namely ultrasonic shear wave tomography, is used to determine presence and extent of voids, honeycombs, cracks perpendicular to the surface, and/or delamination. This technique, and others similar to it, has been utilized in the nuclear industry to determine structural conditions.

14/01427 MRP-227/228 component inspections supporting nuclear power plant license renewal

Renshaw, J. *et al. Energy Conversion and Management*, 2013, 74, 569–573.

As the world's nuclear reactor fleet continues to age, the importance of verifying the structural integrity of critical reactor components and systems has continued to increase. Some critical components are the reactor internals found in close proximity to the nuclear fuel rods which are exposed not only to high stresses and temperatures, but also to high radiation and neutron fluxes. The materials reliability programme (MRP-227/228) has provided guidance indicating which components are of the highest importance and susceptibility to the aging mechanisms found in nuclear reactors. These components must be either inspected or replaced in order for plants to be granted licence renewals to continue commercial operations. Several inspection methods are presented that were successfully demonstrated and comply with these new guidelines to meet the requirements for licence renewal.

14/01428 Nuclear power plant components condition monitoring by probabilistic support vector machine

Liu, J. *et al. Annals of Nuclear Energy*, 2013, 56, 23–33.

In this paper, an approach for the prediction of the condition of nuclear power plant (NPP) components is proposed, for the purposes of condition monitoring. It builds on a modified version of the probabilistic support vector regression (PSVR) method, which is based on the Bayesian probabilistic paradigm with a Gaussian prior. Specific techniques are introduced for the tuning of the PSVR hyerparameters, the model identification and the uncertainty analysis. A real case study is considered, regarding the prediction of a drifting process parameter of a NPP component.

14/01429 Reactor power setback: a procedure to reduce thermal shock on FBR components

Natesan, K. *et al. Annals of Nuclear Energy*, 2013, 56, 7–16.

Fast breeder reactor (FBR) power setback is a procedure to avoid reactor SCRAM for events originating from balance of plant, which do not affect the operation of boiler feed pumps that supply coolant to steam generators. This procedure is envisaged to avoid reactor

components from being subjected to thermal shock due to SCRAM for some of the events that do not affect nuclear safety. In this procedure, all control rods of the reactor are driven down simultaneously to achieve a pre-determined lower power level. Appropriate plant parameters have been identified for the automatic triggering of power setback procedure on the occurrence of those events which are envisaged to be managed through this procedure. Knowledge of the transient thermal hydraulic behaviour of the whole plant during various events is essential to formulate the operating procedure. Plant dynamics code DYANA-P developed for prototype FBRs has been used for this purpose. This paper discusses: (i) events for which this procedure can be adopted, (ii) detailed implantation scheme of power setback, (iii) transient thermal hydraulic behaviour of the whole plant during this procedure and (iv) benefits of this procedure.

14/01430 Recent advances in fusion radioactive material studies

Zucchetti, M. *et al. Fusion Engineering and Design*, 2013, 88, (6–8), 652–656.

This paper focuses on a few recent advances and research developments concerning fusion radioactive waste management studies. The paper considers the role of fusion power in the frame of the future production of nuclear radioactive waste. This is done in terms of potential waste avoidance using a precautionary fusion waste management policy, activation of W and its alloys (examining and comparing the activation of W-based components in ITER, PPCS and ARIES designs), development of a management strategy for activated materials from complex components (such as blanket and diverter), waste decay heat and maintenance questions, materials detritiation, and public acceptance of clearable and recyclable materials.

14/01431 Status of the ITER ion cyclotron H&CD system

Lamalle, P. *et al. Fusion Engineering and Design*, 2013, 88, (6–8), 517–520.

The ongoing design of the ITER ion cyclotron heating and current drive system (20 MW, 40–55 MHz) is rendered challenging by the wide spectrum of requirements and interface constraints to which it is subject, several of which are conflicting and/or still in a high state of flux. These requirements include operation over a broad range of plasma scenarios and magnetic fields (which prompts usage of wide-band phased antenna arrays), high radio-frequency (RF) power density at the first wall (and associated operation close to voltage and current limits), resilience to edge-localized mode-induced load variations, intense thermal and mechanical loads, long pulse operation, high system availability, efficient nuclear shielding, high density of antenna services, remote-handling ability, tight installation tolerances, and nuclear safety function as tritium confinement barrier. R&D activities are ongoing or in preparation to validate critical antenna components (plasma-facing Faraday screen, RF sliding contacts, RF vacuum windows), as well as to qualify the RF power sources and the transmission and matching components. Intensive numerical modelling and experimental studies on antenna mock-ups have been conducted to validate and optimize the RF design. The paper highlights progress and outstanding issues for the various system components.

14/01432 Study on the project of rapid calculation of radiation doses during a nuclear accident in Daya Bay nuclear power plant

Ling, Y. *et al. Energy Procedia*, 2013, 39, 423–427.

A large-scale radiological accident would result in an immediate critical need to assess the radiation doses received by thousands of individuals to allow for prompt and appropriate protective action. To mitigate these risks, a project of rapid calculation of radiation doses during a nuclear accident in Daya Bay nuclear power plant serves as an available resource for the plant, providing tools and services to quickly predict the radiation doses caused by airborne radionuclides, and to provide scientifically based guidance to emergency managers for the protection of human life. This study focuses on developing a programme that can quickly predict the radiation doses according to some special source terms and weather conditions during a nuclear emergency, instead of how to decide the source term, radioactive effluent dispersion model, wind field prediction and diagnosis model and so on. Also, the programme can draw the radiation dose contour on the map within the range of about 20 km around the plant according to the calculation results. The major advantage is that it can be operated easily and is capable of running faster than real time. The majority of accident conditions can be programmed and simulated for predicting the consequences.

14/01433 The effect assessment for fast reactor fuel cycle deployment

Shiotani, H. *et al. Energy Procedia*, 2013, 39, 33–42.

After the Fukushima Dai-ichi nuclear power station accident, the future role and perspectives of the nuclear energy and nuclear fuel cycle are being called into question in Japan. Regarding fast reactor (FR) and related fuel cycle system, the significance of the research, development, demonstration and deployment (RDD&D) of them is also being argued. In this paper the socio-economic effect of the FR cycle deployment was assessed by a combination system of two energy economy models, which are a recursive dynamic computable general equilibrium (CGE) model based on GTAP-E, i.e. an energy environmental version of the Global Trade and Analysis Project (GTAP) model, and a dynamic optimization type energy system model called Dynamic New Earth 21 (DNE21) model to clarify the significance of the RDD&D. Some energy systems, mainly renewable energy such as land/offshore wind, residential/mega solar and battery for power system stabilization as well as innovative nuclear systems under development (i.e. high-temperature gas-cooled reactor systems, and fusion reactor) were added newly to the latest version of the energy economic model for this assessment. Future population and gross domestic product (GDP) base growth rate, energy demand/consumption amount and carbon footprint were important data to describe the future global economic system with the recursive dynamic GTAP-E model. Moreover, potentials to recover resources, innovative technologies, etc. as well as capital costs for power sources, and other energy characteristics were considered to optimize energy supply profiles from the viewpoint of long-term energy system cost minimization through the DNE21 model. The results showed FRs with high economic potential are deployed on a massive scale in Asia and other countries. In addition, the combined analyses of both energy economic models show the promising economic effect by the plentiful inexpensive electricity supply from FRs. In particular, the GDP growth addition in Japan compensates expected RDD&D costs after the several decades from FR deployment. As well as calculating the GDP after the commercial plants' deployment, the socio-economic effects from RDD&D activities were also estimated. The RDD&D of FR is still cost-effective even under the present situation as long as nuclear energy is used continuously.

14/01434 Verification of source term estimation method against measured data for spent fuel hardware characterization

Cho, D.-K. *et al. Annals of Nuclear Energy*, 2013, 58, 36–42.

The Republic of Korea has developed an advanced source term analysis tool, called ASOURCE, to support R&D action plans for the achievement of an advanced fuel cycle employing a pyroprocess in connection with a sodium-cooled fast reactor. ASOURCE has the following functions: (a) generation of inflow and outflow source terms of mixed spent fuel (SF) in each process for the design of the pyroprocess facility; (b) overall inventory estimation for transuranics (TRUs) and long-lived nuclides in SFs stored at each or all reactor sites for the design of the SFR; and (c) grand source terms of a batch of SFs with different irradiation and cooling profiles for the practical design of a temporary or interim storage facility of SFs. ASOURCE is comprised of three analysis sequences, a fuel waste characterization sequence, metal waste characterization sequence, and grand source term characterization sequence. In this study, the metal waste characterization sequence was verified by comparing the nuclide inventory estimated by ASOURCE with the measured nuclide inventory in an irradiated grid plate. It was found that the values calculated by ASOURCE agreed with the measured data within 35%, indicating that the developed program supplies viable source term data.

Economics, policy, supplies, forecasts

14/01435 A new class of indicators for the model selection of scaling laws in nuclear fusion

Lupelli, I. *et al. Fusion Engineering and Design*, 2013, 88, (6–8), 738–741.

The development of computationally efficient model selection strategies represents an important problem facing the analysis of nuclear fusion experimental data, in particular in the field of scaling laws for the extrapolation to future machines, and image processing. In this paper, a new model selection indicator, the model falsification criterion (MFC), will be presented and applied to the problem of choosing the most generalizable scaling laws for the power threshold (P_{Thresh}) to access the H-mode of confinement in tokamaks. The proposed indicator is based on the properties of the model residuals, their entropy and an implementation of the data falsification principle. The model selection ability of the proposed criterion will be demonstrated in comparison with the most widely used frequentist (Akaike information criterion) and Bayesian (Bayesian information criterion) indicators.

14/01436 A nuclear fuel cycle system dynamic model for spent fuel storage options

Brinton, S. and Kazimi, M. *Energy Conversion and Management*, 2013, 74, 558–561.

The options for used nuclear fuel storage location and affected parameters such as economic liabilities are currently a focus of several high-level studies. A variety of nuclear fuel cycle system analysis models are available for such a task. The application of nuclear fuel cycle system dynamics models for waste management options is important to life-cycle impact assessment. The recommendations of the Blue Ribbon Committee on the USA's nuclear future led to increased focus on long periods of spent fuel storage. This motivated further investigation of the location dependency of used nuclear fuel in the parameters of economics, environmental impact, and proliferation risk. Through a review of available literature and interactions with each of the programmes available, comparisons of post-reactor fuel storage and handling options will be evaluated based on the aforementioned parameters and a consensus of preferred system metrics and boundary conditions will be provided. Specifically, three options of local, regional, and national storage were studied. The preliminary product of this research is the creation of a system dynamics tool known as the waste management module which provides an easy-to-use interface for education on fuel cycle waste management economic impacts. Initial results of baseline cases point to positive benefits of regional storage locations with local regional storage options continuing to offer the lowest cost.

14/01437 Detailed evaluation of safety injection tank effects on in-vessel severe accident progression in a small break LOCA without safety injection

Park, R.-J. *et al. Annals of Nuclear Energy*, 2013, 58, 54–59.

The effects of coolant injection into a reactor vessel by the passive actuation of safety injection tanks (SITs) on the in-vessel core melt progression under a severe accident have been evaluated in an advanced power reactor (APR) 1400. A best estimate simulation from initiating events of 2-in. and 3-in. break small break loss coolant accidents (SBLOCAs) without safety injection (SI) to a reactor vessel failure has been carried out using the SCDAP/RELAP5 computer code in conditions with and without the passive actuation of the SITs. The SCDAP/RELAP5 results have shown that the passive coolant injection into the reactor vessel by the actuation of the SITs leads to postpone the reactor vessel failure time by 4–5 h in the SBLOCA without SI. At the time of the reactor vessel failure, 44.5% and 42.8% of the fuel rod cladding were oxidized in the 2-in. and 3-in. SBLOCAs with the actuation of the SITs, respectively. However, 37.5% and 34.6% of the fuel rod cladding were oxidized in the 2-in. and the 3-in. SBLOCAs without the actuation of the SITs, respectively. Even though the SITs are designed for a large break LOCA, their actuation is very effective on the delay of a reactor vessel failure in spite of more hydrogen generation in the SBLOCA without SI.

14/01438 Developments and needs in nuclear analysis of fusion technology

Pampin, R. *et al. Fusion Engineering and Design*, 2013, 88, (6–8), 454–460.

Nuclear analyses provide essential input to the conceptual design, optimization, engineering and safety case of fusion technology in current experiments, ITER, next-step devices and power plant studies. Calculations are intricate and computer-intensive, typically requiring detailed geometry models, sophisticated acceleration algorithms, high-performance parallel computations, and coupling of large and complex transport and activation codes and databases. This paper reports progress on some key areas in the development of tools and methods to meet the specific needs of fusion nuclear analyses. In particular, advances in the production and modernization of reference models, in the preparation and quality assurance of acceleration algorithms and coupling schemes, and in the evaluation and adaptation of alternative transport codes are presented. Emphasis is given to ITER-relevant activities, which are the main driver of advances in the field. Discussion is made of the importance of efforts in these and other areas, considering some of the more pressing needs and requirements. In some cases, they call for a more efficient and coordinated use of the scarce resources available.

14/01439 Evaluating options for the future energy mix of Japan after the Fukushima nuclear crisis

Hong, S. *et al. Energy Policy*, 2013, 56, 418–424.

The Fukushima nuclear accident in March 2011 has increased social and political reluctance to embrace nuclear power in Japan (and elsewhere). The Japanese government has thus been considering four possible future energy mixes, including a nuclear-free pathway, and three others with 10–35% nuclear supply coupled with a larger proportion of renewable energy and fossil fuels to replace nuclear. Here the authors use multi-criteria decision-making analysis (MCDMA) to assess the potential negative economic (levelized cost of electricity, and energy security), environmental (greenhouse gas emissions, land transformation, water consumption, heated water discharge, air pollution, radioactive waste, and solid waste) and social (safety issues) impacts of the four proposed pathways to determine which scenario most holistically minimizes adverse future outcomes. The nuclear-free pathway has the highest overall potential for adverse outcomes (score = 2.49 out of 3), and the 35% nuclear power supply option yielding the lowest negative impact score (0.74) without weightings. Despite some sensitivity to the choice of criterion weights, the analyses demonstrate clearly that from an empirical perspective, a nuclear-free pathway for Japan is the worst option to pursue. The authors recommend that MCDMA methodology used for Japan can be applied to other countries to evaluate future electricity generation scenarios.

14/01440 External costs of nuclear: greater or less than the alternatives?

Rabl, A. and Rabl, V. A. *Energy Policy*, 2013, 57, 575–584.

Since the Fukushima nuclear disaster, many people are calling for a shutdown of nuclear power plants. To see whether such a shutdown would reduce the risks for health and environment, the external costs of nuclear electricity are compared with alternatives that could replace it. The frequency of catastrophic nuclear accidents is based on the historical record, about one in 25 years for the plants built to date, an order of magnitude higher than the safety goals of the US Nuclear Regulatory Commission. Impacts similar to Chernobyl and Fukushima are assumed to estimate the cost. A detailed comparison is presented with wind as alternative with the lowest external cost. The variability of wind necessitates augmentation by other sources, primarily fossil fuels, because storage at the required scale is in most regions too expensive. The external costs of natural gas combined cycle are taken as 0.6 €cent/kWh due to health effects of air pollution and 1.25 €cent/kWh due to greenhouse gases (at €25/t_{CO2eq}) for the central estimate, but a wide range of different parameters is also considered, both for nuclear and for the alternatives. Although the central estimate of external costs of the wind-based alternative is higher than that of nuclear, the uncertainty ranges overlap.

14/01441 Nuclear fuel cycle: which strategy to support a sustainable growth for nuclear energy?

Barbat, J.-D. and Liberge, R. *Energy Procedia*, 2013, 39, 69–80.

Recycling the energy from used fuel and efficiently managing the waste are key factors for a sustainable growth of nuclear energy. Advanced nuclear fuel cycles are often presented as a major step forward compared to the current closed fuel cycle, bringing lower volumes and radio toxicity of waste, an enhanced proliferation resistance, uranium savings and economic benefits. The objective of this paper is to demonstrate that the current closed fuel cycle, based on a proven track record of recycling, has already achieved significant advancement, and represents a very efficient way to prepare for the future implementation of an advanced closed fuel cycle. In the context of post-Fukushima safety analyses, it is also a strong argument to promote the public acceptance of nuclear power development. The overall cost of current closed cycle is about 6% of the kWh cost. It is a competitive solution which reduces financial uncertainties compared to direct disposal. The advantages of the current closed fuel cycle have been demonstrated by the successful policy of recycling implemented in Europe for more than 30 years. With the new AREVA EPR™ reactor, recycling will take another step forward, enabling MOX fuel loading of up to 100%, thus offering additional management options of recycled fuel, and giving more flexibility to its customers.

14/01442 Oxidation behavior analysis of cladding during severe accidents with combined codes for Qinshan Phase II nuclear power plant

Shi, X. *et al. Annals of Nuclear Energy*, 2013, 58, 246–254.

Core behaviour at a high temperature is extremely complicated during transition from design basic accident (DBA) to the severe accident (SA) in light water reactors (LWRs). The progression of core damage is strongly affected by the behaviour of fuel cladding (oxidation, embrittlement and burst). A severe accident programme (SAP) is developed to simulate the process of fuel cladding oxidation, rupture and relocation of core debris based on the oxidation models of cladding, candling of melted material and mechanical slumping of core components. Relying on the thermal–hydraulic boundary parameters calculated by RELAP5 code, analysis of a SA caused by the large break loss-of-coolant accident without mitigating measures for Qinshan phase II nuclear power plant (QSP-II NPP) was performed by SAP for finding the key sequences of accidents, estimating the amount of hydrogen generation and oxidation behaviour of the cladding.

14/01443 Risk assessment of potential catastrophic accidents for transportation of special nuclear materials through Turkish Straits

Bolat, P. and Yongxing, J. *Energy Policy*, 2013, 56, 126–135.

The Turkish Straits region comprises of two straits, Dardanelles and Bosphorus, and the Marmara Sea. It is a historical marine trade route between the former Soviet countries and the western world. From the perspective of special nuclear materials transportation, this route can also be a nuclear materials trade route due to the nuclear policy of former Soviet countries and world nuclear market. In addition, the Turkish Straits can also be an optional route of integrated transportation ways for the shipping states that pursue to reach the destination points using the Black Sea countries or the north-eastern part of Turkey. Consequently maritime transportation of special nuclear materials has arisen as a critical concept for the Turkish Straits, where the risks should be understood and analysed effectively. Accordingly, this study will aim at conducting a risk assessment for the Turkish Straits from the special nuclear material transportations perspective via two hypothesized scenarios: (i) a ship collision accident in the case of special nuclear materials transportation through the Turkish Straits and (ii) a ship fire accident in the case of nuclear smuggling through the Turkish Straits with an oil tanker. These scenarios are modelled and analysed using RADTRAN 5 code and the results presented.

14/01444 Safety analysis code SCTRAN development for SCWR and its application to CGNPC SCWR
Wu, P. *et al. Annals of Nuclear Energy*, 2013, 56, 122–135.
Design analysis is one of the main difficulties during the research and design of SCWRs. Currently, the development of safety analysis code for SCWR is still in its infancy all around the world, and very few computer codes could carry out the trans-critical calculations where significant changes in water properties would take place. In this paper, a safety analysis code SCTRAN for SCWRs has been developed based on code RETRAN-02, the best estimate code used for safety analysis of light water reactors. The ability of SCTRAN code to simulate transients where both supercritical and subcritical regimes are encountered has been verified by comparing with APROS and RELAP5–3D codes. Furthermore, the LOFA and LOCA transients for the CGNPC SCWR design were analysed with SCTRAN code. The characteristics and performance of the passive safety systems applied to CGNPC SCWR were evaluated. The results show that: (1) the SCTRAN computer code developed in this study is capable to perform design analysis for SCWRs; (2) during LOFA and LOCA accidents in a CGNPC SCWR, the passive safety systems would significantly mitigate the consequences of these transients and enhance the inherent safety.

14/01445 Simplified approach for reconstructing the atmospheric source term for Fukushima Daiichi nuclear power plant accident using scanty meteorological data
Oza, R. B. *et al. Annals of Nuclear Energy*, 2013, 58, 95–101.
The atmospheric source term for the Fukushima Daiichi nuclear power plant accident in March 2011 has been estimated by a Gaussian puff based atmospheric dispersion model. The scanty meteorological data available at irregular time intervals are utilized to demonstrate the utility of such data along with a simplified modelling approach to derive useful information. The source terms for I-131 and Cs-137 have been estimated as a function of time from the observed values of activity concentration in the air and deposited activity on the ground. The model results suggest that during the period from 12 March to 16 March 2011, 9.29×10^{16} Bq of I-131 and 6.15×10^{15} Bq of Cs-137 might have been released to the environment.

14/01446 Site selection considerations of spent nuclear fuel reprocessing plant in China
Wang, B. *et al. Energy Procedia*, 2013, 39, 382–386.
With the conversion of nuclear development strategy from 'proper development' to 'positive development' in China, the future nuclear power scale and the amount of spent nuclear fuel will be enormous, the construction of a spent nuclear fuel reprocessing plant will be necessary to meet the sustainable development requirements. Because of the huge investment and high environmental sensitivity, the site selection has always been the focus of controversy. This article summarizes the site selection considerations from the technical feasibility, safety reliability, environmental compatibility and economic rationality for further discussion about the scientific site selection of spent nuclear fuel reprocessing plant in China.

14/01447 Study on containment safety systems for Korean fusion DEMO plant
Oh, K. *et al. Fusion Engineering and Design*, 2013, 88, (6–8), 648–651.
The purpose of this study is to review the strategy for radiation barriers in the fusion power plants and to produce simulation data for the conceptual design of safety features to maintain the integrity of such barriers as a part of R&D programme through the National Fusion Research Institute of Korea. Even though the amount of radioactive source term in fusion power plants should be much less than that of fission power plants, internal as well as external events can result in damage to facilities such that public can be critically exposed by radiation. In the first part of this study, the authors reviewed and compared the multiple defences to protect radioactive hazard in fission and fusion power plants. Containment was characterized as an indispensable physical barrier and the integrity of containment particularly enveloping a fuel cycle which is a major radioactive source term, tritium, should be secured. Since water is assumed as one of the coolant options in the Korean fusion DEMO plant, the thermo-hydraulic analysis was carried out using computer simulations to produce key parameters related with the integrity of containment in the second part. The performance of both of active and passive safety features to control the key parameters was compared to take recent fission technologies into account.

14/01448 The risk is in the relationship (not the country): political risk management in the uranium industry in Kazakhstan
Conway, J. E. *Energy Policy*, 2013, 56, 201–209.
How do we account for multinational energy companies that are able to operate in 'risky' political environments? While traditional risk indices may tell us why a country is considered a difficult operating environment, they tell us very little about why some multinationals are nevertheless able to operate successfully in such countries over long periods of time. In fact, risk indices by their very nature make 'success' almost impossible to capture due to their sole focus on country behaviour. In reality, when a multinational energy company enters into a given country, the firm establishes relationships with a series of stakeholders, not a single 'host country' entity; further, the behaviours of those stakeholders (good or bad) do not exist in a vacuum, but rather are largely influenced by the multinational's own behaviour. In other words, the risk is in the relationship between the firm and the country's stakeholders. This paper argues that success is therefore a function of the firm's ability to manage relationships among a variety of stakeholders within a given country. A case study of Cameco, a Canadian-based uranium mining multinational which has been operating in the politically 'risky' country of Kazakhstan for two decades, bears this out.

06 ELECTRICAL POWER SUPPLY AND UTILIZATION

Scientific, technical

14/01449 A new cogeneration targeting procedure for total site utility system
Khoshgoftar Manesh, M. H. *et al. Applied Thermal Engineering*, 2013, 54, (1), 272–280.
As a head of design, the cogeneration targeting is necessary to optimal design of site utility in the process industries to estimate fuel demand, steam generation, steam used as well as production of heat and power. A new cogeneration targeting model has been developed to estimate the cogeneration potential of site utility systems. The new procedure has been proposed here provides a consistent, general procedure for determining the mass flow rates and the efficiencies of the turbines used. This algorithm utilizes the relationship of the entropy with the enthalpy and the isentropic efficiency. Finally the new model allows targeting shaft work production and degree of superheat at steam boiler with high accuracy. It is superior to previous works in that it does not require cumbersome simulation for initiation and accurate. Also, this algorithm is simple, clear to understand with high computational efficiency and could be easily to provide computer code rather than simulation programs. Three case studies are used to illustrate the usefulness of the new cogeneration targeting method.

14/01450 A stable adaptive fuzzy control scheme for tracking an optimal power profile in a research nuclear reactor
Rojas-Ramírez, E. *et al. Annals of Nuclear Energy*, 2013, 58, 238–245.
An innovative adaptive fuzzy control scheme for power tracking in a research nuclear reactor is presented. The reference power profile is devised to attain the desired power in the minimum possible time while maintaining the period parameter above the safety limit value at all times. The controller incorporates a group of fuzzy systems to identify the reactor's non-linear dynamics. The Lyapunov stability theory is used to establish a procedure for the adjustment of the fuzzy system free parameters. Likewise, a supervisor stage keeps the power error

within a bounded region. To validate the control scheme, the dynamics of the reactor is modelled by the set of point kinetic equation. The simulation results show the feasibility of using this approach as a new technique to regulate the power in a TRIGA-type research nuclear reactor.

14/01451 A traveling-wave thermoacoustic electric generator with a variable electric R-C load

Sun, D. M. *et al. Applied Energy*, 2013, 106, 377–382.

A travelling-wave thermoacoustic electric generator, which is composed of a travelling wave thermoacoustic engine and linear alternators, is promising in solar power generation and energy recovery due to its high efficiency, high reliability, and capability of utilizing low-grade heat. An equivalent acoustic circuit of a linear alternator is first built and analysed using electro–mechano-acoustical analogy. It is found that the acoustic coupling of the linear alternators to the travelling-wave thermoacoustic engine is crucial to the performance of the system. A travelling-wave thermoacoustic electric generator with a variable electric R-C load is then constructed and experimentally studied. Both the theoretical analysis and the experimental results show the importance of mechanical and electrical resonances to the overall performance of the system. Furthermore, the thermal-to-electric efficiency and the electric power are found to be proportional to the pressure amplitude and the square of it in front of the piston of the linear alternator, respectively. By optimizing the load impedance, the travelling-wave thermoacoustic electric generator has achieved a maximum electric power of 345.3 W with a thermal-to-electric efficiency of 9.34% and a maximum efficiency of 12.33% with an electric power of 321.8 W at around 65 Hz when helium of 3.0 MPa is used as the working gas.

14/01452 Coal chemical-looping combustion for electricity generation: investigation for a 250 MW_e power plant

Authier, O. and Le Moullec, Y. *Energy Procedia*, 2013, 37, 588–597.

Chemical-looping combustion (CLC) is generally based on interconnected fluidized beds where a solid oxygen carrier provides the oxygen for combustion in a fuel reactor (FR). The reduced oxygen carrier is then regenerated to oxidized state in an air reactor (AR) before being recycled to FR to complete the loop. CLC may be suitable and highly promising for power plants with near-zero CO_2 emissions. This paper presents, from process thermodynamic modelling, a theoretical investigation of coal chemical-looping combustion for electricity generation with usual steam cycle. The technical issue of unburned compounds minimization at FR outlet is examined through direct oxygen injection in FR. Heat recovery systems are combined on the one hand with a supercritical seam cycle suited to low corrosivity of depleted air from AR, and on the other hand with a sub-critical steam cycle used in open-loop for steam production to fluidize oxygen carrier in FR and gasify char obtained from coal pyrolysis. The integrated configuration presented at one design point is shown to be promising in terms of net plant efficiency (41.6% LHV) including CO_2 capture and compression.

14/01453 High rate performance activated carbons prepared from ginkgo shells for electrochemical supercapacitors

Jiang, L. *et al. Carbon*, 2013, 56, 146–154.

Partially graphitized ginkgo-based activated carbon (GGAC) is fabricated from ginkgo shells by pyrolysis, KOH activation and heat treatment using cobalt nitrate as graphitization catalyst. The graphitization temperature is 900 °C. The GGAC has a microporous structure and its specific surface area is 1775 $m^2 g^{-1}$. XRD patterns show that the carbon becomes more graphitic after heat treatment. The specific capacitance of the GGAC reaches to 178 $F g^{-1}$ at a potential scan rate of 500 $mV s^{-1}$, which is superior to that of commercial activated carbons and ordered mesoporous carbons. The high electrochemical performance of the GGAC is attributed to its good electronic conductivity and high surface area. Partially graphitized activated carbon is a promising electrode material for electrochemical supercapacitors with high rate performance.

14/01454 Incorporating residential AC load control into ancillary service markets: measurement and settlement

Bode, J. L. *et al. Energy Policy*, 2013, 56, 175–185.

Many pre-existing air conditioner (AC) load control programs can provide valuable operational flexibility but have not been incorporated into electricity ancillary service markets or grid operations. Multiple demonstrations have shown that residential AC response can deliver resources quickly and can provide contingency reserves. A key policy hurdle to be overcome before AC load control can be fully incorporated into markets is how to balance the accuracy, cost, and complexity of methods available for the settlement of load curtailment. Overcoming this hurdle requires a means for assessing the accuracy of shorter-term AC load control demand reduction estimation approaches in an unbiased manner. This paper applies such a method to compare the accuracy of approaches varying in cost and complexity – including regression analysis, load matching and control group approaches – using feeder data, household data and AC end-use data. The authors recommend a practical approach for settlement, relying on an annually updated set of tables, with pre-calculated reduction estimates. These tables allow users to look up the demand reduction per device based on daily maximum temperature, geographic region and hour of day, simplifying settlement and providing a solution to the policy problem presented in this paper.

14/01455 Microbial fuel cells for azo dye treatment with electricity generation: a review

Solanki, K. *et al. Bioresource Technology*, 2013, 131, 564–571.

A microbial fuel cell (MFC) has great potential for treating wastewater containing azo dyes for decolorization, and simultaneous production of electricity with the help of microorganisms as biocatalysts. The concept of MFC has been already well established for the production of electricity; however, not much work has been published regarding dye decolorization with simultaneous electricity generation using MFCs. This paper reviews the performance limitations, future prospects, and improvements in technology in terms of commercial viability of azo dye decolorization with electricity generation in MFC. The major limitation identified is the high cost of cathode catalyst. Therefore, there is need of developing inexpensive cathode catalysts. Biocathode is one such option. Moreover, enhanced performance can be obtained by photo-assisted electrochemical process like rutile-coated cathode.

14/01456 Online VAR support estimation for voltage stability enhancement

Balamurugan, G. and Aravindhababu, P. *International Journal of Electric Power & Energy Systems*, 2013, 49, 408–413.

The existing resources in present-day power systems are inadequate to meet the ever-growing load demand and as a result the grids are operated closer to the voltage stability boundaries. The system is therefore prone to voltage collapse even for a small increase in load demand. VAR support appears to be the only viable remedial measure. This paper develops a fuzzy based online tool to determine the minimum VAR support required for a projected load demand with a view to ensure voltage stability in a power system. The tool incarnates a methodology through which the operator can initiate steps to improve the voltage profile and bring the system far away from the point of voltage collapse. It includes the test results of three IEEE systems to exhibit the viability and effectiveness of the proposed method.

14/01457 Preparation and characterization of high surface area, high porosity carbon monoliths from pyrolyzed bovine bone and their performance as supercapacitor electrodes

Goodman, P. A. *et al. Carbon*, 2013, 55, 291–298.

Bovine cortical bone was pyrolysed to produce a network of conductive carbon entwined with native hydroxyapatite that maintains its macroscopic structure during pyrolysis and prevents collapse of the carbon. Self-supporting conductive carbon monoliths were prepared by removing the hydroxyapatite with acid or ethylenediaminetetraacetic acid. The specific surface areas of these monoliths were determined by nitrogen adsorption, and their chemical structure was characterized using Raman spectroscopy. The monoliths exhibit specific surface areas and Raman spectra similar to those of amorphous carbons. Capacitance was assessed using the monoliths as the working electrodes in three-electrode cells, and two-electrode devices in which both electrodes were monoliths. Individual monoliths exhibit specific capacitances of 134 ± 11 F/g in aqueous solutions of potassium nitrate and 108 ± 9 F/g in the ionic liquid 1-ethyl-3-methylimidizolium bis(trifluoromethylsulfonyl)imide. The capacitance of individual 6 mm diameter by 1 mm thick electrodes was typically on the order of 0.2 F.

14/01458 Promoting energy-saving and environmentally friendly generation dispatching model in China: phase development and case studies

Ding, Y. and Yang, H. *Energy Policy*, 2013, 57, 109–118.

Energy saving and environmental protection are important conditions for the sustainable development of Chinese economy. However, current widely used generation scheduling model based on predefined production quota and tariff results in heavy energy consumption and severe environment pollution. From 2007, as concerns over energy shortage and environmental pollution, the Chinese authorities introduced the implementation of energy-saving generation dispatching model, which is an important approach to facilitating energy-saving and reduction of pollutant emission. The objective of implementing energy-saving generation dispatching model is to prioritize the use of renewable energy resources and new power plants with high efficiency without compromising power system security and reliability. This paper analyses the necessity and feasibility of implementing energy-efficient and environmentally friendly generation scheduling models in China. The institutional and technical barriers impeding the implementation of energy-saving generation dispatching model are identified. The

development of advanced energy-saving generation scheduling models towards competitive market models and phased planning programmes are emphasized in this paper. The effectiveness and experience of provinces' piloted energy-saving generation dispatching projects are also discussed.

14/01459 Synthesis of large area carbon nanosheets for energy storage applications

Cott, D. J. *et al. Carbon*, 2013, 58, 59–65.

This paper reports the large area growth of highly conductive carbon nanosheets (CNS) composed of few layer graphene on 200 mm diameter Si substrates using conventional radio frequency plasma-enhanced chemical vapour deposition. Raman spectroscopy is used to characterize the evolution of the CNS nucleation and growth with time in conjunction with TEM revealing the nano-sized graphene-like nature of these films and the intimate contact to the substrate. An individual sheet can have edges as thin as three graphene layers. The influence of the growth support layer is also discussed as film growth is compared on titanium nitride (TiN) and directly on Si. Electrochemical cyclic voltammogram (CV) measurements reveal these layers to form an excellent electrical contact to the underlying substrate with excellent stability towards oxidation while having a large electrochemical surface area. The resistance of a 150 nm film was measured to be as low as 20 μΩ cm. The high percentage of narrow few layer graphene edge sites exposed allows for faster electrochemical reaction rates compared to carbon nanotubes and other electrode materials (glassy carbon and Pt).

14/01460 Thermodynamic analysis of pumped thermal electricity storage

White, A. *et al. Applied Thermal Engineering*, 2013, 53, (2), 291–298.

The increasing use of renewable energy technologies for electricity generation, many of which have an unpredictably intermittent nature, will inevitably lead to a greater need for electricity storage. Although there are many existing and emerging storage technologies, most have limitations in terms of geographical constraints, high capital cost or low cycle life, and few are of sufficient scale (in terms of both power and storage capacity) for integration at the transmission and distribution levels. This paper is concerned with a relatively new concept which will be referred to here as pumped thermal electricity storage (PTES), and which may be able to make a significant contribution towards future storage needs. During charge, PTES makes use of a high temperature ratio heat pump to convert electrical energy into thermal energy which is stored as 'sensible heat' in two thermal reservoirs, one hot and one cold. When required, the thermal energy is then converted back to electricity by effectively running the heat pump backwards as a heat engine. The paper focuses on thermodynamic aspects of PTES, including energy and power density, and the various sources of irreversibility and their impact on round-trip efficiency. It is shown that, for given compression and expansion efficiencies, the cycle performance is controlled chiefly by the ratio between the highest and lowest temperatures in each reservoir rather than by the cycle pressure ratio. The sensitivity of round-trip efficiency to various loss parameters has been analysed and indicates particular susceptibility to compression and expansion irreversibility.

Economics, policy, supplies, forecasts

14/01461 A case study of a cogeneration system for a hospital in Greece. Economic and environmental impacts

Alexis, G. K. and Liakos, P. *Applied Thermal Engineering*, 2013, 54, (2), 488–496.

The objective of the present work is to investigate whether the Tzaneio hospital, located in Piraeus, Greece, is a potential candidate for the implementation of a cogeneration system and also to determine the most suitable cogeneration system (electricity and heat). More specifically, after the presentation of the hospital's energy consumption and the calculation of the energy consumption costs, alternative energy scenarios have been examined that propose the installation of cogeneration units of different power capacity for various profiles of operational hours. A comparative evaluation has been carried out for the selection of the most suitable CHP unit, following a specific procedure and taking into account a number of critical factors. The study showed that when the main gas engine (diesel with natural gas) operates 8000 h/year and the backup unit 5000 h/year, the cogeneration system is most economically profitable. The total annual energy cost has been reduced by 32.4%. The benefit to cost ratio is greater than one, the net present value is positive and the internal rate return for 20-year lifetime of system is 19%. Also there is reduction of annual primary energy consumption by 28%, as well as a significant annual reduction of pollutant emissions.

14/01462 A cost-benefit analysis of generating electricity from biomass

O'Mahoney, A. *et al. Energy Policy*, 2013, 57, 347–354.

A key challenge internationally is the design of future electricity systems which will bring about emissions savings and fuel security at least cost. Peat is used to generate electricity in several European Union countries, mainly to take advantage of indigenous resources and increase fuel mix diversity. The Irish government has introduced a target of 30% co-firing of peat and biomass by 2015. This paper assesses the feasibility of achieving this target by calculating the available indigenous biomass resource capable of being co-fired; the cost of meeting the target; the benefits in terms of carbon abatement; and finally the present value in economic terms of meeting the target. Results demonstrate that Ireland has only half the necessary resource to meet the 30% target and that the net cost of doing so is greater than the cost of what is currently being paid for peat, in all of the scenarios considered. Thus, it is concluded that while it may be technically possible to meet the target by combining national resources with imported biomass this is never the least cost option, and as a result the targeted focus of Government policy may need to be reconsidered.

14/01463 Costs and benefits of the renewable production of electricity in Spain

Burgos-Payán, M. *et al. Energy Policy*, 2013, 56, 259–270.

The reduction of pollutant emissions and greenhouse gases, as well as the strong energy dependence on fossil fuels (gas and fuel oil), have, among other reasons, led many countries in recent years to develop policies to promote and encourage the use of alternative, sustainable, clean and predictable sources of energy. This paper presents an overview of the production of electricity from renewable sources in Spain, and offers an outline of the current level of development of renewable energy. It also reviews the current support system, the costs of integrating renewable energy into the electric system as well as the effects of this type of energy on the electricity wholesale market price, the gross domestic product, the environment, human health and employment.

14/01464 Day-ahead electricity prices forecasting by a modified CGSA technique and hybrid WT in LSSVM based scheme

Shayeghi, H. and Ghasemi, A. *Energy Conversion and Management*, 2013, 74, 482–491.

At the present time, day-ahead electricity market is closely associated with other commodity markets such as fuel market and emission market. Under such an environment, day-ahead electricity price forecasting has become necessary for power producers and consumers in the current deregulated electricity markets. Seeking for more accurate price forecasting techniques, this paper proposes a new combination of a feature selection technique-based mutual information technique and wavelet transform. Moreover, a new modified version of gravitational search algorithm optimization-based chaos theory, namely the chaotic gravitational search algorithm (CGSA) is developed to find the optimal parameters of least square support vector machine (LSSVM) to predict electricity prices. The performance and price forecast accuracy of the proposed technique is assessed by means of real data from price markets in Iran, Ontario and Spain. The simulation results from numerical tables and figures in different cases show that the proposed technique increases electricity price market forecasting accuracy than the other classical and heretical methods in the scientific researches.

14/01465 Distributed optimal power flow for smart grid transmission system with renewable energy sources

Lin, S.-Y. and Chen, Y.-F. *Energy*, 2013, 56, 184–192.

This study proposes a distributed and parallel optimal power flow (DPOPF) algorithm for a smart grid transmission system with renewable energy sources to account for the fast variation of the power generated by renewable energy sources. The proposed DPOPF algorithm is a combination of the recursive quadratic programming method and the Lagrange projected gradient method; it can achieve the complete decomposition and can be executed in the smart grid transmission system to make distributed and parallel computation possible. Petri nets are also proposed to control the computational synchronization of the DPOPF algorithm under the asynchronous data arrival in the smart grid transmission system. The proposed DPOPF algorithm is applied to solve optimal power flow problems in a smart grid transmission system with renewable energy sources on a 26-bus test system. The test results demonstrate the computational efficiency of the proposed DPOPF algorithm, which is fast enough to cope with the fast variation of the power generated by renewable energy sources, and justify the accuracy of the obtained solutions.

14/01466 Energetic and exergetic efficiencies of coal-fired CHP (combined heat and power) plants used in district heating systems of China

Liao, C. *et al. Energy*, 2013, 57, 671–681.

The efficiencies of coal-fired combined heat and power (CHP) plants used in the district heating systems of China were analysed with a thermodynamic model in the Hysys program. The influences of four parameters were evaluated by the Taguchi method. The results indicated that the extraction steam flow rate and extraction steam pressure are the most important parameters for energetic and exergetic efficiencies, respectively. The relations between extraction steam flow rate, extraction steam pressure and the energetic and exergetic efficiencies were investigated. The energetic and exergetic efficiencies were compared to the relative primary energy savings (RPES) and the relative avoided irreversibility (RAI). Compared to separate heat and power (SHP) generation, the CHP systems save fuel energy when extraction ratio is larger than 0.15. In the analysis of RAI, the minimum extraction ratio at which CHP system has advantages compared with SHP varies between 0.25 and 0.6. The higher extraction pressure corresponds to a higher value. Two of the examined plants had design conditions giving RPES close to zero and negative RAI. The third had both positive RPES and RAI at design conditions. The minimum extraction ratio can be used as an indicator to design or choose CHP plant for a given district heating system.

14/01467 Environmental efficiency analysis of power industry in China based on an entropy SBM model

Zhou, Y. *et al. Energy Policy*, 2013, 57, 68–75.

In order to assess the environmental efficiency of power industry in China, this paper first proposes a new non-radial data envelopment analysis approach by integrating the entropy weight and the slack-based model (SBM). This will improve the assessment reliability and reasonableness. Using the model, this study then evaluates the environmental efficiency of the Chinese power industry at the provincial level during 2005–2010. The results show a marked difference in environmental efficiency of the power industry among Chinese provinces. Although the annual, average, environmental efficiency level fluctuates, there is an increasing trend. The Tobit regression analysis reveals the innovation ability of enterprises, the proportion of electricity generated by coal-fired plants and the generation capacity have a significantly positive effect on environmental efficiency. However, the waste fees levied on waste discharge and investment in industrial pollutant treatment are negatively associated with environmental efficiency.

14/01468 Experimental evaluation of a real time energy management system for stand-alone microgrids in day-ahead markets

Marzband, M. *et al. Applied Energy*, 2013, 106, 365–376.

A microgrid (MG) energy management system (EMS) is a key supervisory control tool to make decisions regarding the best use of the electric power generation resources and storage devices within this MG. This paper presents an operational architecture for the real-time operation (RTO) of an islanded MG. Two different parts of the architecture are considered, the central control unit (CCU) and MG testbed. The CCU implements an EMS based on the local energy market (LEM) to control a MG. In order to reach this objective, this unit executes day-ahead scheduling (DAS) and real-time scheduling (RTS). Regarding DAS, a modified conventional EMS (MCEMS) based on the LEM ($MCEMS_{-LEM}$) algorithm has been proposed to find out hourly power set-points of distributed energy resources (DERs) and customers. LEM is also presented in $MCEMS_{-LEM}$ to obtain the best purchasing price in day-ahead market, as well as to maximize the utilization of existing DER. With regard to RTS, it must update and feedback the power set-points of DER by considering the results of DAS. The presented architecture is flexible and could be used for different configurations of MGs also in different scenarios. Simulations and experimental evaluations have been carried out using real data to test the performance and accuracy of the MG testbed. This paper aims to operate the MG in islanded mode, ensuring uninterruptable power supply services and reducing the global cost of generated power. The results demonstrate the effectiveness of the proposed algorithm and show a reduction in the generated power cost by almost 8.5%.

14/01469 Fuel electricity and plug-in electric vehicles in a low carbon fuel standard

Yang, C. *et al. Energy Policy*, 2013, 56, 51–62.

Electricity is unique among the alternative fuels in a low carbon fuel standard (LCFS) policy, in that demand from vehicles is the major barrier to its usage, not supply. This paper presents a policy discussion and policy recommendations on a number of topics related to the regulation and incentives for fuel electricity within the LCFS. In the near-term, the LCFS will have a limited role in incentivizing the use of electricity and lowering the carbon intensity of electricity, and electricity will play a small role in meeting LCFS targets. Calculating a carbon intensity value for electricity is a complex process, requiring many decisions and trade-offs to be made, including allocation methods, system boundaries, temporal resolution and how to treat electricity demand for vehicle charging. These choices along with other regulatory decisions about who can obtain LCFS credits will influence the incentives for providing electricity and charging infrastructure relative to other low-carbon fuels as well as across different electricity providers. The paper discusses how fuel electricity would fit into an LCFS, identifying those special characteristics that could reduce the effectiveness of the policy. It also provides specific recommendations to enable better policy design that appropriately incentivizes the use of low-carbon fuels.

14/01470 Impacts of compressed air energy storage plant on an electricity market with a large renewable energy portfolio

Foley, A. and Lobera, I. D. *Energy*, 2013, 57, 85–94.

Renewable energy generation is expected to continue to increase globally due to renewable energy targets and obligations to reduce greenhouse gas emissions. Some renewable energy sources are variable power sources, for example wind, wave and solar. Energy storage technologies can manage the issues associated with variable renewable generation and align non-dispatchable renewable energy generation with load demands. Energy storage technologies can play different roles in each of the step of the electric power supply chain. Moreover, large-scale energy storage systems can act as renewable energy integrators by smoothing the variability. Compressed air energy storage is one such technology. This paper examines the impacts of a compressed air energy storage facility in a pool-based wholesale electricity market in a power system with a large renewable energy portfolio.

14/01471 Institutional work and climate change: corporate political action in the Swedish electricity industry

Sarasini, S. *Energy Policy*, 2013, 56, 480–489.

This paper uses qualitative methods to examine factors that influence corporate political actions (CPA) linked to climate policy in the Swedish electricity industry. CPA strategies are examined in connection to two policy instruments – the European Union's emission-trading scheme and the Swedish electricity certificate scheme. These instruments are the main drivers of climate-related investments in the sector. The study treats CPA as a form of institutional work and examines reasons for companies to seek to maintain/disrupt institutions. The study finds that CPA is driven primarily by the need to manage external resource dependencies and that where risks are more acute, companies are more likely to seek to disrupt regulative institutions. However, the study also shows that respondents' appraisals of policy instruments are based on a convergent set of shared values (cognitive institutions) that form the basis of CPA and which actors do not seek to disrupt despite resource-based risks. CPA is thus characterized as a means to transmute cognitively held values and beliefs into regulative institutions. The study concludes with implications for policymakers and theory.

14/01472 Investigating the link between well-being and energy use; an explorative case study between passive and active domestic energy management systems

Pelenur, M. J. and Cruickshank, H. J. *Building and Environment*, 2013, 65, 26–34.

The aim of this study was to explore how the remote control of appliances/lights (active energy management system) affected household well-being, compared to in-home displays (passive energy management system). A 6-week exploratory study was conducted with 14 participants divided into the following three groups: active, passive, and no equipment. The effect on well-being was measured through thematic analysis of two semi-structured interviews for each participant, administered at the start and end of the study. The well-being themes were based on existing measures of satisfaction and affect. The energy demand for each participant was also measured for 2 weeks without intervention, and then compared after 4 weeks with either the passive or active energy management systems. These measurements were used to complement the well-being analysis. Overall, the measure of affect increased in the passive group but satisfaction decreased; however, all three measures on average decreased in the active group. The measured energy demand also highlighted a disconnect between well-being and domestic energy consumption. The results point to a need for further investigation in this field; otherwise, there is a risk that nationally implemented energy management solutions may negatively affect happiness and well-being.

14/01473 Methods for detailed energy data collection of miscellaneous and electronic loads in a commercial office building

Lanzisera, S. *et al. Building and Environment*, 2013, 65, 170–177.

Miscellaneous and electronic loads (MELs) consume about 20% of the primary energy used in US buildings, and this share is projected to increase for the foreseeable future. The understanding, however, of which devices are most responsible for this energy use is still

rudimentary due to the difficulty and expense of performing detailed studies on MELs and their energy use. In order to better understand the energy use of MELs and the design of MELs field metering studies, a year-long study of MELs was conducted in an 89,500 sq. ft (8310 m^2) office building. The authors present insights obtained from this study using 455 wireless plug-load power meters including the study design process, the tools needed for success, and key other methodology issues. The study allowed the authors to quantify, for the study buildings, how many devices were needed to inventory and meter as well as for how long meter data should be collected. The authors found that the study design of earlier work would not have yielded accurate results in the study building. This paper presents these findings along with a brief summary of the energy related results.

14/01474 Nuclear fusion and renewable energy forms: are they compatible?

Hamacher, T. *et al. Fusion Engineering and Design*, 2013, 88, (6–8), 657–660.

Nuclear fusion can be considered as a base-load power plant technology: high investment costs and limited operational flexibility require continuous operation. Wind and solar, on the other hand, as the putative main pillars of a future renewable energy system, are intermittent power sources. The resulting variations that occur on many different time scales require at first sight a rather flexible back-up system to balance this stochastic behaviour. Fusion would appear not to be well suited for this task. The situation changes, however, if a large-scale renewable energy system is envisaged based on a transnational, or even transcontinental power grid. The present paper discusses a possible European power system in the year 2050 and beyond. A high percentage share of renewable energies and a strong power grid spanning the whole of Europe and involving neighbouring countries, in particular those in north Africa, are assumed. The linear programming model URBS is used to describe the power system. The model optimizes the overall system costs and simulates power plant operation with an hourly resolution for one whole year. The geographical resolution is at least at the country level. The renewable technologies are modelled first on a more local level and then summed together at the country or regional level. The results indicate that the smoothing effects of the large-scale power grid transform the intermittent renewable supply, which is then more compatible with base-load power plants such as fusion reactors.

14/01475 Occupants interaction with electric lighting and shading systems in real single-occupied offices: results from a monitoring campaign

da Silva, P. C. *et al. Building and Environment*, 2013, 64, 152–168.

This study presents the results of a monitoring campaign aiming to further the understanding of occupants' behaviour regarding the manual control of electric lighting in combination with shading control. It was performed on eight single-occupied offices in the city of Porto, Portugal, during periods ranging from 28 to 60 days per office. A wide range of environmental variables including workplane illuminance, window and background luminance and transmitted solar radiation was measured with high frequency (20 min time steps). The study aimed to address a set of key research questions regarding typical illuminance ranges, luminance distribution and occupancy patterns found in offices and their relationship to electric lighting or shading control actions. It also enabled to compare observed behaviour with predictions from benchmarking behavioural models found in the literature. The main findings were that electric lighting and shading control were influenced more by occupational dynamics (arrival and departure) than by the environmental conditions experienced over the day (daylight workplane illuminance or transmitted solar radiation), though with a large degree of variability between occupants and/or offices. It also revealed that while most of the behavioural models analysed for comparison purposes were in qualitative agreement with field observations (e.g. more lighting switch-on actions at arrival for lower daylight illuminances), only one model (Pigg's model) predicted the frequency of observed lighting switch-off events. These findings strongly support the need for more numerous (and geographically more broadly distributed) office behaviour monitoring campaigns to increase the robustness of such models.

14/01476 Potential of structural thermal mass for demand-side management in dwellings

Reynders, G. *et al. Building and Environment*, 2013, 64, 187–199.

In order to avoid grid instability and decreasing production efficiencies of large power plants due to a widespread integration of renewable electricity production, demand-side management (DSM) is proposed as a solution to overcome the possible mismatch between demand and supply. This research evaluates the potential to improve the balance between the electricity use for heating and local electricity production of a nearly zero energy building (nZEB), by active use of structural thermal storage capacity of the building. To quantify the DSM potential of structural thermal storage, the cover factors and peak electricity demand of a single family dwelling equipped with a photovoltaic (PV) system are chosen. Detailed representations of the PV system and the dwelling itself, heated by an air–water heat pump, are implemented in the modelling environment of Modelica and simulated for the heating-dominated climate of Belgium. The influence of the insulation level and the embedded thermal mass of the construction on the DSM potential is evaluated. The impact of the heat emission system is estimated by comparing a floor heating system with a radiator emission system. Results show that although the influence on the cover factors is limited, the use of the structural storage capacity for demand-side management shows strong potential to shift the peak electricity use for heating to off-peak hours. Furthermore, it is shown that not only the availability of the thermal mass, but also the interaction between the heating system and the thermal mass is of significant importance.

14/01477 Review of challenges in reliable electric power delivery to remote deep water enhanced oil recovery systems

Narayanaswamy, V. *Applied Ocean Research*, 2013, 43, 53–67.

This paper reviews the major challenges involved in reliable electric power delivery to remote deep water enhanced oil recovery (EOR) systems. As the oil well matures, top side based booster systems are not economical, and hence, subsea based booster systems are required. Such EOR processes require subsea systems to be operated at varying power and voltage levels, and this requires establishing subsea power stations with long tiebacks from the shore. Subsea stations carry out safe voltage step-down, distribution and conversion of electrical power in the order of megawatts. Breakdowns in subsea based EOR systems lead to huge production losses, and system retrieval for repair and maintenance is very costly and time consuming, and therefore systems need to be highly reliable. This paper describes the technical challenges involved in subsea variable speed motor drives, long step out power transmission, subsea energy storage requirements for safe start up and emergency shutdown, thermal and humidity management inside pressure rated enclosures, fault localization, pressure-tolerant electronics and bio-fouling. Emerging advancements in electrical, power electronic, power transmission, energy storage and packaging technologies are reviewed, giving the confidence that the present technical maturity would be able to drive the development of reliable subsea based EOR systems.

14/01478 Short-term electric load and temperature forecasting using wavelet echo state networks with neural reconstruction

Deihimi, A. *et al. Energy*, 2013, 57, 382–401.

In this paper, wavelet echo state network (WESN) with a novel echo state network (ESN)-based reconstruction stage is applied to both short-term load forecasting (STLF) and short-term temperature forecasting (STTF). Wavelet transform is used as the front stage for multi-resolution decomposition of load or temperature time series. ESNs function as forecasters for decomposed components. A modified shuffled frog leaping algorithm is used for optimizing ESNs. Both 1-h and 24-h ahead predictions are studied where the number of inputs are kept minimum. The performance of the proposed WESN-based load forecasters are investigated for three cases as the predicted temperature input is fed by actual temperatures, output of the WESN-based temperature forecasters and noisy temperatures. Effects of temperature errors on load forecasts are studied locally by sensitivity analysis. Hourly loads and temperatures of a North American electric utility are used for this study. First, results of the proposed forecasters are compared with those of ESN-based forecasters that have previously shown high capability as stand-alone forecasters. Next, the WESN-based forecasters are compared with other models either previously tested on the data used here or to be rebuilt for testing on these data. Comparisons reveal significant improvements on accuracy of both STLF and STTF using the proposed forecasters.

14/01479 Structural reform of Japanese electric power industry: separation between generation and transmission & distribution

Goto, M. *et al. Energy Policy*, 2013, 56, 186–200.

This study examines the cost structure of Japanese electric power industry to investigate whether a structural reform on the industry really enhances a cost-saving benefit to consumers. A composite cost function model, using a panel data set, is used for this study. The data set consists of nine electric power companies from 1990 to 2008. Based on the estimation results, this study examines whether economies of scale and vertical economies exist in the industry. Then, this study conducts a cost subadditivity test that is a necessary condition of natural monopoly. The empirical results indicate that the electric power firms exhibit the status of economies of scale in their transmissions and distributions and the operation as a whole. However, they do not exhibit economies of scale in their generations. Thus, the transmission operation, by integration, in a large area can improve its

economic efficiency. Furthermore, the industry should introduce more competition in both generation and wholesale power markets where more firms can participate in their power trades. This study also empirically confirms that vertical economies have existed in the industry. Moreover, this study confirms that all the estimates in the cost subadditivity test satisfy the necessary condition of natural monopoly, where each estimate indicates cost saving in cost subadditivity. The test does not guarantee a sufficient condition of natural monopoly. However, it clearly indicates that the functional separation between generation and transmission will increase total production cost in the industry. The complete separation may result in a net loss of economic efficiency if a competition benefit does not exceed an expected economic loss. Consequently, this study suggests that the industrial structure of future Japanese electric power industry should be evaluated from not only an expected benefit by introducing competition but also an unbundling cost that occurs with a loss of vertical integration.

14/01480 The deployment of electricity generation from renewable energies in Germany and Spain: a comparative analysis based on a simple model
Fernández, P. F. *et al. Energy Policy*, 2013, 57, 552–562.
The fulfilment of the aims set by the European Union in the deployment of renewable energy sources for electricity generation (RES-E) has counted and must continue to count on public funding from the member states, which promote private investment in this type of facilities. This funding guarantees a cost-oriented remuneration which, being higher than the market price means an additional cost to the electricity system. With the aim of minimizing the economic impact as the weight of RES-E in the electricity mix increases, the generation costs of renewable units must approach those of the market, which are expected to increase according to the fossil fuel price forecasts. The present study analyses both the RES-E development and deployment in Spain and Germany, two pioneering countries worldwide and with very similar electricity systems. Based on their national action plans and a simple model, this analysis approaches the RES-E surcharge, comparing and contrasting the results obtained in both countries.

14/01481 The looming revolution: how photovoltaics will change electricity markets in Europe fundamentally
Haas, R. *et al. Energy*, 2013, 57, 38–43.
The increase in photovoltaic (PV) capacities in Germany, since 2011, has, on some days, already significant impacted spot market prices at the German electricity exchange. The core objective of this paper is to investigate the possible effects of a further uptake of PV on the prices in electricity markets. Two major effects are analysed: (i) the direct impact of PV at specific times of the year when PV shifts the supply curve of conventional electricity virtually out of the market, leading to temporarily very low market prices close to zero; (ii) the indirect impact of PV (and wind) on the costs at which fossil capacities are offered at times when renewable energy sources are scarce. The major effects of these developments on the electricity markets will be: (i) a much higher price volatility from hour to hour and day to day; (ii) higher prices for electricity from fossil capacities and storage technologies for balancing the intermittent renewable generation; and (iii) growth of balancing markets and intensified competition at the level of decentralized balancing organizations.

07 STEAM RAISING

Boiler operation/design

14/01482 Arch- and wall-air distribution optimization for a down-fired 350 MW_e utility boiler: a cold-modeling experimental study accompanied by real-furnace measurements
Kuang, M. *et al. Applied Thermal Engineering*, 2013, 54, (1), 226–236.
To determine the effect of the arch- and wall-air distribution on flow characteristics, experiments were conducted within a 1 : 15-scaled model for a down-fired 350 MW_e furnace at various settings, i.e. ratios (denoted by R_d) of the mass flow rate of staged air to that of total secondary air of 0%, 7%, 16%, 23% and 29%. Meanwhile, industrial scale measurements were performed at full load with staged-air damper openings of 15% and 35% (equal to R_d at about 10% and 20%), respectively. At settings of $R_d = 0\%$ and 7%, an essentially symmetric flow field appeared. At the left three higher settings (i.e. $R_d = 16\%$, 23% and 29%), a deflected flow field developed, with the airflow near the front wall penetrating much further than that near the rear wall. At this time, increasing R_d deteriorates the flow-field deflection. By means of cold-modelling experiments to evaluate the flow-field symmetric extent and downward airflow penetration depths in the lower furnace, the appropriate R_d was found to be in the range of 7–16%. Real-furnace measurements revealed that although the 15% opening was inapplicable in boiler operations for a long time, relatively symmetric combustion could developed at the this opening setting. At the 35% opening setting, an asymmetric combustion pattern developed in the furnace, with temperatures near the front wall being clearly higher that those near the rear wall. However, particularly high NO_x emissions and good burnout developed at both two openings. In considering that numerical simulations and industrial scale measurements in published work have confirmed the validity of a previously-proposed deep-air-staging combustion technology in achieving excellent furnace performance within down-fired furnaces, retrofitting the present furnace with the technology is thus recommended if symmetric combustion, good burnout, and low NO_x emissions are to be achieved.

14/01483 CFD prediction of mixing in a steam generator mock-up: comparison between full geometry and porous medium approaches
Dehbi, A. and Badreddine, H. *Annals of Nuclear Energy*, 2013, 58, 178–187.
In computational fluid dynamics (CFD) simulations of single-phase flow mixing in a steam generator (SG) during a station blackout severe accident, the problem occurs of representing the thousands of SG U-tubes. Typically, simplifications are made to render the problem computationally tractable. In particular, one or a number of tubes are lumped in one volume that is treated as a single porous medium which replicates the pressure loss and heat transfer characteristics of the real tube. This approach significantly reduces the computational size of the problem and hence simulation time. This study investigates the adequacy of this approach by performing a series of simulations. The porous medium approach is first validated against results of the one-seventh scale Westinghouse SG–S3 test. In a second step, two separate simulations are made of flow in the PSI SG mock-up, i.e. one in which the porous medium model is used for the tube bundle, and another in which the full geometry is represented. In all simulations, the Reynolds Stress model of turbulence is used. The authors show that in steady state conditions, the porous medium treatment yields results that are comparable to those of the full geometry representation (temperature distribution, recirculation ratio, hot plume spread, etc.). Hence, the porous medium approach can be extended with a good degree of confidence to model single phase mixing in the full-scale SG.

14/01484 Exergetic sustainability analysis of LM6000 gas turbine power plant with steam cycle
Aydin, H. *Energy*, 2013, 57, 766–774.
The aim of this study is to develop the exergetic sustainability indicators in order to determine sustainability aspects of gas turbine engine (GTE) based power plant. For this purpose, first a comprehensive exergy analysis of GTE is carried out then the exergetic sustainability indicators are calculated for two power plant configuration, case A for LM6000 GTE-based power plant, case B for LM6000 GTE-based power plant with steam turbine cycle. The investigated exergetic sustainability indicators are exergy efficiency, waste exergy ratio, exergy destruction factor, recoverable exergy ratio, environmental effect factor and exergetic sustainability. At maximum power operation, case A power plant generates 43.3 MW electricity power whereas 54.3 MW of electricity power is generated by case B power plant thanks to steam turbine cycle contribution. Results show that exergetic sustainability index is obtained as 0.651 for case A and 0.978 for case B power plant. Steam turbine cycle results in improvement of overall efficiency and reviewed exergetic sustainability indicators evidently. Decrease of waste exergy ratio leads to decrease of environmental effect factor and increase both exergetic efficiency and exergetic sustainability index. Moreover, studying these parameters indicates how much improvement is possible for GTE to achieve better sustainability.

14/01485 Experimental study on combustion and NO_x emissions for a down-fired supercritical boiler with multiple-injection multiple-staging technology without overfire air
Kuang, M. *et al. Applied Energy*, 2013, 106, 254–261.
A deep-air-staging combustion technology was previously developed to achieve reduction in NO_x emissions and to eliminate strongly asymmetric combustion found in down-fired boilers. Recently, one of two down-fired 600 MW_e supercritical utility boilers using this technology (without applying overfire air) began commercial operations. To understand coal combustion and NO_x emissions characteristics within the furnace, full-load industrial-size experiments were performed at different air-staging conditions with measurements taken of gas temperatures in the burner region, gas temperatures and species

concentrations in the near wing-wall region, carbon content in fly ash, and NO_x emissions. As expected, the furnace performance characterized by relatively timely coal ignition, symmetric combustion, and low levels of carbon in fly ash, developed in the furnace at all three settings. Deepening the air-staging conditions could reduce NO_x emissions by one-fifth, but varied slightly carbon in fly ash. In view of the still high NO_x production (i.e. 1036 mg/m^3 at 6% O_2), adding an overfire air system which was essentially a part of the technology, was recommended for the boiler to significantly reduce the present NO_x emissions.

14/01486 Implementation and rejection of industrial steam system energy efficiency measures
Therkelsen, P. and McKane, A. *Energy Policy*, 2013, 57, 318–328.
Steam systems consume approximately one-third of energy applied at US industrial facilities. To reduce energy consumption, steam system energy assessments have been conducted on a wide range of industry types over the course of 5 years through the Energy Savings Assessment (ESA) programme administered by the US Department of Energy. ESA energy assessments result in energy efficiency measure recommendations that are given potential energy and energy cost savings and potential implementation cost values. Saving and cost metrics that measure the impact recommended measures will have at facilities, described as percentages of facility baseline energy and energy cost, are developed from ESA data and used in analyses. Developed savings and cost metrics are examined along with implementation and rejection rates of recommended steam system energy efficiency measures. Based on analyses, implementation of steam system energy efficiency measures is driven primarily by cost metrics: payback period and measure implementation cost as a percentage of facility baseline energy cost (implementation cost percentage). Stated reasons for rejecting recommended measures are primarily based on economic concerns. Additionally, implementation rates of measures are not only functions of savings and cost metrics, but time as well.

14/01487 Influence of fuel particle size on gasification in a dual fluidized bed steam gasifier
Wilk, V. and Hofbauer, H. *Fuel Processing Technology*, 2013, 115, 139–151.
The influence of the distribution of fuel particle size on steam gasification was studied systematically in a dual fluidized bed gasifier. Pilot plant gasification experiments have been conducted using sawdust and pellets produced from the same raw material. Three different kinds of waste wood with a broad particle size distribution were also considered for comparison. The fuels differ in their content of particles smaller than 1 mm of equivalent diameter. With an increasing proportion of particles smaller than 1 mm, the product gas contained less H_2 and more CO and CH_4. Less product gas was generated and the concentration of tar increased. It is observed that entrainment of small fuel particles plays an important role in the dual fluidized bed gasifier. Based on the superficial gas velocity in the freeboard of the gasification reactor, a limiting diameter for the entrainment of fuel particles can be determined. Under the conditions investigated a total of 22 wt% of fuel particles present in the mixture of sawdust and pellets was entrained very rapidly after feeding because of their size. They mainly devolatilize in the freeboard and only have limited contact with the catalytic bed material. Therefore, these volatiles are less likely to be reformed and more tar is found in the product gas. As a conclusion, the particle size determines the region where the thermal conversion of the fuel particle mainly takes place: within the fluidized bed or in the freeboard.

14/01488 Numerical study of a 350 MWe tangentially fired pulverized coal furnace of the As Pontes power plants
Constenla, I. *et al. Fuel Processing Technology*, 2013, 116, 189–200.
This investigation aims to predict the flow characteristics with real operating conditions of a boiler in order to understand the phenomena occurring in the interior of the furnace and to validate the models chosen for the simulation. For this purpose, the authors carried out a numerical study of the flow of a reactive gas mixture with pulverized coal combustion occurring in a tangentially fired furnace of a real power plant. These calculations were developed with the commercial software ANSYS Fluent. Furthermore, a home-made code was built to perform some necessary preprocessing and post-processing calculus. In particular, this code solves zero-dimensional balances that have provided a good agreement with the calculated and measured flow at the exit of the furnace and it is also used to validate the convergence of the numerical algorithm for the three-dimensional simulation. The results obtained from this study show that models and numerical methods selected are appropriate to correctly predict the combustion processes within the furnace. In conclusion, the validation of this numerical model and the home-made code provides the user a complete tool to evaluate the performance of a boiler under different operating conditions, reducing the cost of experimental tests.

14/01489 Shape and operation optimisation of a supercritical steam turbine rotor
Nowak, G. and Rusin, A. *Energy Conversion and Management*, 2013, 74, 417–425.
The presented study discusses the problem of shape optimization of selected areas of the rotor of the high pressure part of an ultra-supercritical steam turbine together with the optimization of the turbine start-up method, using the maximum stress objective. The analysis relates to the rotor of a conceptual ultra-supercritical turbine which is characterized by high parameters of operation. The consequence is that the machinery components are subjected to significant stress, which further results in a substantial reduction in its life and reliability. These adverse effects can be contained in two ways, i.e. by optimizing the shape of the rotor areas characterized by high stress values and by optimizing the method of the turbine start-up. In the case of the rotor under analysis, it is the thermal stress caused by large temperature gradients occurring in unsteady states of operation that has a predominant impact on the stress level. The performed research shows that the manner in which the power unit start-up is initiated and carried out depends largely on the limitations of the materials used to make the machinery components. This, in turn, has an impact on the assessment of the power unit in terms of energy and economy. The obtained optimization results translate directly into the power unit energy effectiveness.

08 COMBUSTION

Burners, combustion systems

14/01490 A comparative evaluation of gray and non-gray radiation modeling strategies in oxy-coal combustion simulations
Nakod, P. *et al. Applied Thermal Engineering*, 2013, 54, (2), 422–432.
Computational fluid dynamic simulations of oxy-coal combustion are demonstrated in a lab-scale furnace and full-scale boiler employing gray and non-gray formulations of recently proposed radiative property models for the gas-phase. The investigated scenarios included: air-firing, oxy-firing with dry and wet flue-gas recycle (FGR). The study confirms that the temperature and wall radiative flux profiles encountered during air firing can be replicated in both dry and wet FGR scenarios through an appropriate selection of $(CO_2 + H_2O)/O_2$ molar ratios in the oxidizer stream. The computed temperature profiles were in reasonable agreement with the experimental measurements. In the lab-scale furnace, lower flame temperatures and smaller path lengths minimized the differences between the gray and non-gray model predictions. Within the full-scale boiler, large volume pockets were present where the radiation was dominated by the gas-phase. This combined with higher peak flame temperatures and longer path lengths resulted in: a 10% variation between the gray and non-gray radiative fluxes and a 50 K difference in the predicted average outlet gas temperatures.

14/01491 A layer-by-layer deposition mechanism for producing a pyrolytic carbon coating on carbon nanotubes
Zheng, G.-B. *et al. Carbon*, 2013, 57, 267–273.
Pyrolytic carbon (PyC) was deposited on carbon nanotubes (CNTs) in order to modify them by introducing defects to their surface. The deposition of PyC was carried out at temperature between 800 and 1000 °C using propane as carbon source with or without a hydrogen carrier gas at low pressure of 20 kPa. The structure of PyC coatings was examined using transmission electron microscopy. The PyC coating could be distinguished from the original CNT walls due to the difference of the structure, with the coating showing a less orderly layer structure. When H_2 was introduced during deposition, PyC coating started to form at 900 °C, and the deposition rate increased rapidly with increasing temperature. Without H_2, PyC coating with a thickness of a few layers could be formed at temperatures between 800 and 900 °C in 10 min. The outmost layer of the PyC coating showed a structure of rough and curved carbon fragment. A layer-by-layer mechanism is proposed for the deposition consisting of alternating fragment formation (nucleation) and lateral growth to layer.

14/01492 A study of slow pyrolysis of one low rank coal via pyrolysis–GC/MS
Lievens, C. *et al. Fuel Processing Technology*, 2013, 116, 85–93.

This paper describes the study of one low rank coal (LRC). To investigate its molecular structure, a LRC was characterized by proximate and ultimate analyses, XRD, FTIR, Raman spectroscopy, and pyrolysis–GC/MS (py–GC/MS). The light volatile fraction of LRC was characterized via py–GC/MS. The LRC's aromatic ring structures consist of 59% amorphous structures, 22% of highly ordered structures with no less than six rings, 16% of aromatic structures characterized by aliphatic and/or ether substitutions and 3% of substituted benzene rings. XRD results show that the crystalline unit of LRC contains 1.44 aromatic carbon atoms per aliphatic carbon atom. Aromatic cluster structures within LRC are interconnected via ether and covalent C–C bonds. Hydroxyl, ether and carbonyl functionalities give the LRC its polar character. The slow pyrolysis of the LRC resulted in a light volatile GC/MS detected fraction consisting of 20% aromatic ring compounds, 45% of phenolics, 30% of aliphatic hydrocarbons and 5% O-compounds, of which the concentration, evolution and nature were dependent on the heating rates and end temperatures. Generally, slow pyrolysis of LRC at 700 °C yielded the highest concentrations of unsaturated acyclic hydrocarbons, aromatics and phenolics.

14/01493 Amino acid salts for CO_2 capture at flue gas temperatures

Wei, S. C.-C. *et al. Energy Procedia*, 2013, 37, 485–493.

An amino acid salt, potassium taurate, has been chosen as a high-temperature absorbent in this study due to its low volatility and high absorption rate. The densities and viscosities of 2M-6 M taurate solution have been determined over the temperature range from 293 to 353 K. The CO_2 solubility of taurate solutions has been measured using a stirred-cell reactor. It has been found that the CO_2 solubility of taurate solutions is comparable to that of alkanolamines at high temperature. The absorption rate of CO_2 into CO_2-free and CO_2-loaded taurate solutions were obtained using a wetted-wall column. The K_G of 4 M taurate at 353 K is similar in magnitude to the K_G of 5 M MEA at 313 K. It has also been found that the K_G of taurate decreased with increased CO_2 loading, but the values for K_G of taurate solutions are still comparable to CO_2-loaded 5 M MEA solution.

14/01494 Characterisation of spruce, salix, miscanthus and wheat straw for pyrolysis applications

Butler, E. *et al. Bioresource Technology*, 2013, 131, 202–209.

This research details the characterization of four Irish-grown lignocellulosic biomasses for pyrolysis by biomass composition analysis, TGA, and Py-GC/MS-FID. Ash content (mf) increased in the order spruce (0.26 wt%) < salix (1.16 wt%) < miscanthus (3.43 wt%) < wheat straw (3.76 wt%). Analysis of hydrolysis-derived sugar monomers showed that xylose concentrations (4.69–26.76 wt%) ranged significantly compared to glucose concentrations (40.98–49.82 wt%). Higher hemicellulose and ash contents probably increased non-volatile matter, and decreased the temperature of maximum degradation by TGA as well as yields of GC-detectable compounds by Py-GC/MS-FID. Differences in composition and degradation were reflected in the pyrolysate composition by lower quantities of sugars (principally levoglucosan), pyrans, and furans for salix, miscanthus, and wheat straw compared to spruce, and increased concentrations of cyclopentenones and acids.

14/01495 Co-combustion characteristics and blending optimization of tobacco stem and high-sulfur bituminous coal based on thermogravimetric and mass spectrometry analyses

Zhang, K. *et al. Bioresource Technology*, 2013, 131, 325–332.

Despite much research on co-combustion of tobacco stem and high-sulfur coal, their blending optimization has not been effectively found. This study investigated the combustion profiles of tobacco stem, high-sulfur bituminous coal and their blends by thermogravimetric analysis. Ignition and burnout performances, heat release performances, and gaseous pollutant emissions were also studied by thermogravimetric and mass spectrometry analyses. The results indicated that combustion of tobacco stem was more complicated than that of high-sulfur bituminous coal, mainly shown as fixed carbon in it was divided into two portions with one early burning and the other delay burning. Ignition and burnout performances, heat release performances, and gaseous pollutant emissions of the blends present variable trends with the increase of tobacco stem content. Taking into account the above three factors, a blending ratio of 0–20% tobacco stem content is conservatively proposed as optimum amount for blending.

14/01496 Combustion characteristics of hydrogen-rich alternative fuels in counter-flow diffusion flame configuration

Safer, K. *et al. Energy Conversion and Management*, 2013, 74, 269–278.

Fuels containing large amounts of hydrogen have combustion properties highly depending on composition, in particular hydrogen concentration, and operating conditions such as pressure. A thorough understanding of strained laminar flames is a prerequisite to achieve improved knowledge of more complex system involving hydrogen-rich alternative fuels. This paper reports a numerical investigation of syngas counter-flow diffusion flame structure and emissions over a wide range of operating conditions (H_2/CO ratio between 0.4 and 2.4 and an ambient pressure of 1–10 atm). Special attention is focused on optimal operating conditions in regard to NO_x emissions and NO_x reactions pathways. Flame structure is characterized by solving flamelet equations with the consideration of radiation. The chemical reaction mechanism adopted is GRI-Mech 3.0. Computational results showed that flame structure and emissions are impacted by syngas composition and ambient pressure. The maximum flame temperature exhibits a peak at an intermediate scalar dissipation rate for a given value of H_2/CO ratio. For values of strain rate lower than the intermediate value, flame structure is influenced by combined effects of adiabatic temperature and radiation heat loss, whereas only adiabatic temperature effect prevails at higher values of strain rate. The flame temperature increases more the syngas is H_2-rich for strain rates values below the intermediate value. The opposite behaviour is noticed at strain rate values higher than the intermediate value. NO_x formation is closely related to flame temperature. Hydrogen-rich syngas flames produce more NO_x at lower strain rates while NO_x levels increase towards hydrogen-lean syngas flames at higher strain rates. Zeldovich route is found to be the main NO_x formation route and its contribution to the NO_x production continually increases with H_2 content and pressure.

14/01497 Effect of atmospheric stability on the impact of domestic wood combustion to air quality of a small urban township in winter

Grange, S. K. *et al. Atmospheric Environment*, 2013, 70, 28–38.

In the winter of 2011, a field campaign was undertaken in the small township of Nelson, New Zealand to measure the vertical and horizontal distribution of concentrations of airborne particulate matter. The aim of this campaign was to improve the understanding of the causal factors which result in periods of very high concentrations of particulate pollution in small townships during winter where emissions are dominated by the combustion of wood for domestic heating. The results showed that mean hourly surface concentrations of particulates throughout the airshed were characterized by a distinctive diurnal cycle, with two peaks in concentration (one in the late evening and then, unusually, a second mid-morning). Although the timing and magnitude of hourly peak concentrations was variable throughout the valley, there was no evidence to suggest that regional or topographic flows played a significant role in the build-up of pollutants at any given location. Analysis of vertical profiles of black carbon showed that high concentrations of particulates were confined to the lowest 50 m of the boundary layer. Concentrations decreased with increasing height within this polluted surface layer. The atmosphere was very stable during the evening period. After midnight, a period of increased mixing was consistently identified throughout the lowest 100 m of the boundary layer and associated with the sudden cleansing of the surface and lower layers of the boundary layer. Throughout the observational period there was no evidence for the storage of pollutants aloft. Thus the vertical mixing of pollutants to the surface could not account for increased pollutant concentrations during the morning period. However, at this time the boundary layer remained stable and concentrations of black carbon were mixed through a very shallow layer. This suggests that despite lower domestic heating emissions in the morning, the reduced mixing volume is a likely cause of the observed marked peak in morning surface concentrations.

14/01498 Effect of fuel–air mixture velocity on combustion instability of a model gas turbine combustor

Yoon, J. *et al. Applied Thermal Engineering*, 2013, 54, (1), 92–101.

Nowadays, it is easy for unstable combustion phenomenon to develop in a gas turbine that is working in a lean premixed condition. To eliminate the onset of these instabilities and develop effective approaches for control, the mechanisms responsible for their occurrence must be understood. The flame recirculation zone is very important, as it can modulate the fuel flow rate and may be the source of instability, plus its flame structure has a major impact on heat release rate oscillation and flame stabilization. In this study, experiments were conducted under various operating conditions with a model gas turbine combustor to examine the relation of combustion instability and flame structure by OH chemiluminescence. A swirling CH_4–air flame was investigated with an overall equivalence ratio of 1.2 to lean blowout limit and dump plane velocity of 30–70 m/s. Phase-locking analysis was performed to identify structural changes at each phase of the reference dynamic pressure sensor under conditions of instability. At an unstable condition, flame root size varies a lot compared to stable condition which is because of air and fuel mixture flow rate changes due to combustor pressure modulation. After this structural change, local extinction and re-ignition occur and it can generate a feedback loop for combustion instability. This analysis suggests that pressure fluctuation of combustion causes deformation of flame structure and variation of flame has a strong effect on

combustion instability. In this study, two types of combustion instability characteristics were observed related to the instability of both the thermo-acoustic and flame vortex type.

14/01499 Effect of high-frequency alternating electric fields on the behavior and nitric oxide emission of laminar non-premixed flames

Zhang, Y. *et al. Fuel*, 2013, 109, 350–355.

This paper examined the behaviour and NO emission of laminar non-premixed methane/air jet flames when subjected to high frequency alternating electric fields of 10 kHz over the voltage range of 0–4.0 kV. In particular, this paper examined variations of flame shape and luminosity, CO and NO molar fractions in the downstream flue gas, and chemiluminescence from OH* and CH* in the voltage-influenced flame zone. The results showed that with no application of an alternating electric field, flames were stable at the nozzle exit, bluish at the base and yellowish at the conical tip. However, once applied, different voltage regimes produced different responses from the flame. In the low-voltage regime of 0–1.0 kV, increasing the voltage narrowed the top yellowish zone of the flame and sharpened its conical tip, increased the CO molar fraction in the flue gas, decreased the NO molar fraction in the flue gas, and decreased the chemiluminescence intensity of OH* and CH* in the flame zone by ~50%. At 1.0 kV, both CO and NO molar fractions reached extreme values, and the flame was at its weakest. In the mid-voltage regime of 1.0–3.0 kV, increasing the voltage resulted in an inverse response from the flames compared to the low-voltage regime. In the high-voltage regime of 3.0–4.0 kV, increasing the voltage resulted in the gradual disappearance of the top yellowish zone of the flame, increased the CO molar fraction in the flue gas and decreased the NO molar fraction. The transition mechanisms between the regimes are discussed within the context of the high-frequency discharge theory. Three competing effects explain the non-monotonic flame response to the voltage: thermal, ionic wind, and electrical–chemical. The analysis showed that the ionic wind effect majored in the low-voltage regime, the electrical–chemical effect dominated the mid-voltage regime, and all three effects were highly coupled in the high-voltage regime.

14/01500 Effects of ethanol–diesel–biodiesel blends on combustion and emissions in premixed low temperature combustion

Fang, Q. *et al. Applied Thermal Engineering*, 2013, 54, (2), 541–548.

In this study, the effect of ethanol on combustion and emissions in premixed low temperature combustion (LTC) was investigated in a four cylinders heavy-duty diesel engine. The biodiesel was used as an additive to prevent the stratification of ethanol and diesel blends. The premixed LTC is achieved by the medium level of exhaust gas recirculation and the prolonged ignition delay. Compared with diesel fuel, ethanol–diesel–biodiesel blends have lower NO_x emissions due to lower combustion temperature, resulting from the higher latent heat of vaporization. Unfortunately, the lower combustion temperature also leads to the higher HC and CO emissions. Smoke emissions for ethanol blends decrease obviously because of higher oxygen content and longer ignition delay. The oxygen in ethanol also has a favourable impact on the reduction of smoke emissions, which is obvious in high loads. Thus, the upper load limit of LTC mode is extended. Compared with diesel fuel, 20 vol.% ethanol in diesel and biodiesel blends (BDE20) has lower NO_x and smoke emissions and higher brake thermal efficiency in LTC.

14/01501 Experimental investigation on gaseous emissions from the combustion of date palm residues in laboratory scale furnace

El may, Y. *et al. Bioresource Technology*, 2013, 131, 94–100.

Emissions characteristics from the combustion of five date palm residues (DPR) (date palm leaflets, date palm rachis, date palm trunk, date stones and fruit stalk prunings) in a laboratory-scale furnace were investigated. Release of gaseous products such as CO_2, CO, VOC, NO_x and SO_2 were measured at 600–800 °C. The main goal was to analyse the thermal behaviour and gaseous emissions in order to select the most convenient biofuel for an application in domestic boiler installations. Regards to biofuel characteristics, date stones have the highest energy density (11.4 GJ/m^3) and the lowest ash content (close to 1.2%). Combustion tests show that among the tested date palm residues, date stones may be the promising biofuel for the design of combustion processing system. However, special attention should be given to the design of the secondary air supply in order to prevent high emissions of CO and volatile matter.

14/01502 Experimental investigations on effects of wall-temperature on performance of a pulse detonation rocket engine

Wang, K. *et al. Experimental Thermal and Fluid Science*, 2013, 48, 230–237.

To study the effects of wall-temperature on performance of a pulse detonation rocket engine (PDRE), long-duration experiments were conducted. An internally grooved semi-circle spiral, instead of traditional Shchelkin spiral, was utilized to facilitate the deflagration to detonation transition (DDT) process and prolong run time in the present study. Four pressure transducers and a type K thermocouple were employed to collect data during the experiments. Experiments were carried out at three different operating frequencies, such as 10, 20 and 30 Hz, until unstable operation occurred. The results showed that wall-temperature increased faster at higher operating frequency. It was observed that DDT time and DDT distance both decreased with the increase of wall-temperature, and detonation pressure increased sharply with wall-temperature first and then decreased slowly when wall-temperature exceeded a certain value. Both of them were believed to be due to the impact of hot-wall on fuel vaporization and reactant temperature. Unreasonably high wall-temperature was found to cause pre-ignition of fuel–oxidizer mixture, and this was why unstable operation of the PDRE happened after long-duration runs. In addition, effects of wall-temperature on specific impulse was also discussed.

14/01503 Feasibility of identifying leaking fuel rods using gamma tomography

Holcombe, S. *et al. Annals of Nuclear Energy*, 2013, 57, 334–340.

In cases of fuel failure in irradiated nuclear fuel assemblies, causing leakage of fission gasses from a fuel rod, there is a need for reliable non-destructive measurement methods that can determine which rod is failed. Methods currently in use include visual inspection, eddy current, and ultrasonic testing, but additional alternatives have been under consideration, including tomographic gamma measurements. The simulations covered in this report show that tomographic measurements could be feasible. By measuring a characteristic gamma energy from fission gasses in the gas plenum, the rod-by-rod gamma source distribution within the fuel rod plena may be reconstructed into an image or data set which could then be compared to the predicted distribution of fission gasses, e.g. from the STAV code. Rods with significantly less fission gas in the plenum may then be identified as leakers. Results for rods with low fission gas release may, however, in some cases be inconclusive since these rods will already have a weak contribution to the measured gamma-ray intensities and for such rods there is a risk that a further decrease in fission gas content due to a leak may not be detectable. In order to evaluate this and similar experimental issues, measurement campaigns are planned using a tomographic measurement system at the Halden boiling water reactor.

14/01504 Flue gas cleanup using the moving-bed copper oxide process

Pennline, H. W. and Hoffman, J. S. *Fuel Processing Technology*, 2013, 114, 109–117.

The use of copper oxide on a support had been envisioned as a gas clean-up technique to remove sulfur dioxide (SO_2) and nitric oxides (NO_x) from flue gas produced by the combustion of coal for electric power generation. In general, dry, regenerable flue gas clean-up techniques that use a sorbent can have various advantages, such as simultaneous removal of pollutants, production of a saleable by-product, and low costs when compared to commercially available wet scrubbing technology. Due to the temperature of reaction, the placement of the process into an advanced power system could actually increase the thermal efficiency of the plant. The moving-bed copper oxide process is capable of simultaneously removing sulfur oxides and nitric oxides within the reactor system. In this regenerable sorbent technique, the use of the copper oxide sorbent was originally in a fluidized bed, but the more recent effort developed the use of the sorbent in a moving-bed reactor design. A pilot facility or life-cycle test system was constructed so that an integrated testing of the sorbent over absorption/regeneration cycles could be conducted. A parametric study of the total process was then performed where all process steps, including absorption and regeneration, were continuously operated and experimentally evaluated. The parametric effects, including absorption temperature, sorbent and gas residence times, inlet SO_2 and NO_x concentration, and fly ash loadings, on removal efficiencies and overall operational performance were determined. Although some of the research results have not been previously published because of previous collaborative restrictions, a summary of these past findings is presented in this communication. Additionally, the potential use of the process for criteria pollutant removal in oxy-firing of fossil fuel for carbon sequestration purposes is discussed.

14/01505 Growth of branched carbon nanotubes with doped/un-doped intratubular junctions by one-step co-pyrolysis

Goswami, G. K. *et al. Carbon*, 2013, 56, 97–102.

Branched carbon nanotubes with nitrogen doped/un-doped intratubular junctions have been synthesized by a simple one-step co-pyrolysis of hexamethylenetetramine and benzene. The difference in the vapour

pressure and the insolubility of the precursors are the keys for the formation of the branched intratubular junctions. The junctions behave like Schottky diodes with nitrogen-doped portion as metal and undoped portion as *p*-type semiconductor. The junctions also behave like *p*-type field effect transistors with a very large on/off ratio.

14/01506 Laminar flame speeds of transportation-relevant hydrocarbons and jet fuels at elevated temperatures and pressures

Hui, X. and Sung, C.-J. *Fuel*, 2013, 109, 191–200.

Laminar flame speeds of several fuel/air mixtures were experimentally determined over equivalence ratios of $\Phi = 0.7$–1.3, preheat temperatures of $T_u = 350$–470 K, and pressures of $P = 1$–3 atm in a high-pressure counterflow setup. Fuels investigated in this work included neat components relevant to liquid transportation fuels, such as *n*-decane, *n*-dodecane, *iso*-octane, toluene, *n*-propylbenzene, 1,2,4-trimethylbenzene, and 1,3,5-trimethylbenzene, a conventional Jet-A labelled as POSF 4658, an alternative jet fuel, S-8, labelled as POSF 4734 and a four-component Jet-A surrogate composed of *n*-dodecane, *iso*-octane, *n*-propylbenzene and 1,3,5-trimethylbenzene. The experimental results were also compared with computed values obtained by using various published kinetic models for different fuels. In general, the simulated results are in fair agreement with the experimental data, considering the uncertainties in both experiments and kinetic models. Further analysis on experimental data was conducted to assess the effects of preheat temperature on laminar flame speed and pressure on mass burning flux. From the variation of mass burning flux with pressure, the overall reaction orders of various fuels were extracted. The present flame propagation data at elevated pressures for large hydrocarbons can be used in surrogate formulation and mechanism validation for liquid transportation fuels.

14/01507 Numerical analysis of effect of ignition methods on flame behavior during passing through a sudden contraction near the quenching conditions

Gutkowski, A. *Applied Thermal Engineering*, 2013, 54, (1), 202–211.

The present study numerically investigates the propagation of a laminar premixed propane–air flame in various tubes with a sudden contraction and isothermal cold walls in the stoichiometric mixture. Two different ignition methods are examined: plane and round shaped ignition. These investigations show that for relatively small tubes, the method of ignition does not influence the final flame shape in the tube – it is mushroom-shaped. For wider tubes and the plane ignition method, the flame transforms to a tulip-shaped one. The numerical results show that a flame can enter a smaller diameter tube from a wider one and propagate in a stable manner in all configurations of diameters of both tubes as long as the diameter of the narrow tube is far from the quenching diameter. Decreasing the diameter of the narrow tube, the conditions are approached where the dimension of the wide tube determines if the flame will propagate or quench. This is associated with a temporarily increased ratio of heat losses to thermal energy generation caused by a greater heat loss area. It is also shown that a tulip-shaped flame occurring at large diameters of the wide tube is particularly exposed to quenching during propagation through the sudden contraction.

14/01508 Pressurized oxy-coal combustion: ideally flexible to uncertainties

Zebian, H. and Mitsos, A. *Energy*, 2013, 57, 513–529.

Simultaneous multi-variable gradient-based optimization with multi-start is performed on a 300 MWe wet-recycling pressurized oxy-coal combustion process with carbon capture and sequestration, subject to uncertainty in fuel, ambient conditions, and other input specifications. Two forms of flue gas thermal recovery are studied, a surface heat exchanger and a direct contact separation column. Optimization enables ideal flexibility in the processes: when changing the coal utilized, the performance is not compromised compared to the optimum performance of a process specifically designed for that coal. Similarly, the processes are immune to other uncertainties like ambient conditions, air flow, slurry water flow, atomizer stream flow and the oxidizer stream oxygen purity. Consequently, stochastic programming is shown to be unnecessary. Close to optimum design, the processes are also shown to be insensitive towards design variables such as the areas of the feedwater heaters. Recently proposed thermodynamic criteria are used as embedded design specifications in the optimization process, rendering it faster and more robust.

14/01509 Self-heating co-pyrolysis of excessive activated sludge with waste biomass: energy balance and sludge reduction

Ding, H.-S. and Jiang, H. *Bioresource Technology*, 2013, 133, 16–22.

In this work, co-pyrolysis of sludge with sawdust or rice husk was investigated. The results showed that the co-pyrolysis technology could be used to dispose of the excessive activated sludge without external energy input. The results also demonstrated that no obvious synergistic effect occurred except for heat transfer in the co-pyrolysis if the co-feeding biomass and sludge had similar thermogravimetric characteristics. The experimental results combined with calculation showed that adding sawdust accounting for 49.6% of the total feedstock or rice husk accounting for 74.7% could produce bio-oil to keep the energy balance of the co-pyrolysis system and self-heat it. The sludge from solar drying bed can be further reduced by 38.6% and 35.1% by weight when co-pyrolysed with rice husk and sawdust, respectively. This study indicates that sludge reduction without external heat supply through co-pyrolysis of sludge with waste biomass is practically feasible.

14/01510 Sensitivity analysis of three-parallel-DAEM-reaction model for describing rice straw pyrolysis

Cai, J. *et al. Bioresource Technology*, 2013, 132, 423–426.

The three-parallel distributed activation energy model (DAEM)-reaction model was used to study the slow pyrolysis kinetics of rice straw based on thermogravimetric analysis data. The kinetic parameters of the model were calculated using the pattern search method. A comparison between the predicted derivative thermogravimetric data and experimental values showed good agreement. The influences of the kinetic parameters on the model for describing the experimental data of rice straw were analysed by means of local parametric sensitivity analysis. The results indicated that the frequency factor and the mean value of the activation distribution for cellulose decomposition affect the model more strongly than other parameters, followed by the corresponding parameters for hemicellulose and lignin. The sensitivity of the model to the standard deviations of the activation energy distributions for all pseudocomponents is very slight.

14/01511 Thermal distributive blast furnace gas characterisation, a steelworks case study

Pugh, D. *et al. Applied Thermal Engineering*, 2013, 53, (2), 358–365.

Blast furnace gas (BFG) is a dynamic by-product gas produced in large quantities with a composition comprising typically 18–23% CO, 1–5% H_2 and balance of N_2 and CO_2. Industrial operations lead to fluctuations in gas characteristics over short time periods. This can dissuade engineers from using the gas in increasingly complex technologies with perceived efficiency improvements such as gas turbines, a trait exacerbated by the 'dirty' nature synonymous with industrial process gases. This body of work used the Tata Port Talbot integrated steelworks as a case study to analyse variation in gaseous composition, as a foundation for evaluation of the combustion dynamics associated with BFG. Varying levels of compositional fluctuation were observed, with H_2 providing the most significant contributing factor to fuel characteristic. Particulate contamination was also studied as the gas cools and is distributed around the works, using condensate analyses at multiple distances from source. Particulate loading analyses yielded values of 0.04–0.1 mg N m^{-3} at a distance of over 1.5 km from source, with results implying BFG is thermally scrubbed of contaminant matter through a mechanism of gas cooling and the amalgamation of condensate. The work performed therefore suggests the location of any installed equipment offers a significant contributory factor to performance.

Fire safety

14/01512 Carbon emissions in Mediterranean shrubland wildfires: an experimental approach

Garcia-Hurtado, E. *et al. Atmospheric Environment*, 2013, 69, 86–93.

Forest fire emissions modify the chemical composition of the atmosphere and the Earth's climate system. The Ayora burning experiment was designed to assess and quantify fire emissions from Mediterranean shrublands. A number of gaseous pollutants and particulate matter metrics (CO_2, CO, CH_4, $PM_{2.5}$) were measured during three burning replicates by using real-time monitors. Quantification of carbon emissions released during the experiments showed that 71% was CO_2, 26% CO, 3% CH_4, and only 0.3% was particulate carbon. Emission factors obtained for CO_2, CO and CH_4 were 1257 ± 40, 453 ± 28 and 46 ± 12 g kg^{-1} dry matter, respectively, and combustion efficiencies ranged from 0.46 to 0.99. The experiments allowed the estimation of carbon emission in the different fire phases. Thus, 25% of carbon was sampled in the flaming phase and 75% of C in the smouldering phase. Current natural greenhouse gas emission inventories in Mediterranean countries underestimate the actual emissions from forest fires since they do not consider forest shrub understory and shrublands and since they assume that the CO_2 emitted is offset by forest re-growth. The results may be used to improve current forest-fire emission inventories in southern Europe with special emphasis on shrublands.

14/01513 Heat protection by different phase change materials

Bühler, M. *et al. Applied Thermal Engineering*, 2013, 54, (2), 359–364.
Different types of phase change materials (PCMs) were compared for the use in heat protective clothing. For that purpose, flexible blister foils containing the PCMs were prepared. The samples were irradiated with a heat flux of 1.5 kW/m^2 in order to simulate a typical industrial setting like working in front of a hot oven. The temperature evolution behind the foils indicated the performance of each PCM, which was dependent on the duration of the exposure. For irradiation times up to 9 min, sodium acetate trihydrate lead to the lowest temperature increase and thus the best protection. When irradiating more than 9 min, a zeolite type was found to be more suitable, which lead to a lower temperature increase of up to 36 °C compared to a reference with no PCM. A simple heat transfer model was developed, taking account of the latent heat of the PCM, of the heat capacity of the foil and of the radiant and natural convective heat flow, which could be applied to predict the effect of PCM containing foils and will be used for further optimizations.

14/01514 Hydrogen hazard and mitigation analysis in PWR containment

Şahin, S and Sarwar, M. S. *Annals of Nuclear Energy*, 2013, 58, 132–140.
This paper describes the analytical results for the estimation of hydrogen concentration in the containment atmosphere based on zirconium oxidation reaction following a severe accident. The analysis provides useful information about the potential challenge of local hydrogen accumulation in the containment, which may be used to reduce the hydrogen detonation risk and to design the capacity and arrangements of mitigation measures. The containment analysis has been performed using computer code COGAP that uses the scenario of loss of coolant accident. The behaviour of pressure and hydrogen concentrations in containment as a function of time under the severe accident condition is presented in graphical form. The mitigation measures (recombiners) are essential to maintain containment atmosphere in the safe stable conditions. A hydrogen control system is to mitigate the hydrogen risk by comparing results from a reference accident sequence with and without recombiners. This comparison show that combustible gas occur in few local areas in the containment for a limited time span and hydrogen concentration is reduced significantly with the use of recombiners.

14/01515 Influence of bend structure on high-temperature flow after gas explosion

Pang, L. *et al. Experimental Thermal and Fluid Science*, 2013, 49, 201–205.
In order to study on the influence of bend structures on high-temperature flow of gas explosion in laneways/tubes, a set of experimental facility for gas explosion in tubes with bend structures of different angles and a transient temperature and pressure test system were set up, with the help of which, the variation process of unsteady temperature field when high-temperature flow of methane–air explosion going through the bend structure was studied. The study results show that the bend structure has little influence on high-temperature flow before the bend and has relatively great influence on that after the bend. The bigger the bend angle is, the greater the thermal loss at the bend will be and then the greater the temperature attenuation of the high-temperature flow going through the bend structure will be. In addition, the attenuation of peak temperature after the bend compared with that of corresponding location in the straight tube presents a linear distribution with the bend angle. The above conclusions provide reference basis for compound hazard effect assessment of gas explosion in a complex structure as well as corresponding accident investigation and analysis.

14/01516 Methane emissions from 2000 to 2011 wildfires in northeast Eurasia estimated with MODIS burned area data

Vasileva, A. and Moiseenko, K. *Atmospheric Environment*, 2013, 71, 115–121.
Estimates of methane wildfire emissions from north-east Eurasia for the years 2000–2011 are reported on the basis of satellite burned area data from the moderate resolution imaging spectroradiometer (MODIS MCD45 data product) and ecosystem-dependent fire emission parameters. Average (with standard deviations) emissions are 1.0 ± 0.2 Tg CH_4 year^{-1}, with interannual variations of 0.4–2.3 Tg CH_4 year^{-1}. Most of the emissions are located within 48–55°N, in the southern part of the boreal forest zone, mostly in Siberia and the Far East. The largest discrepancies among independent present-day estimates are found in the sub-polar regions of West Siberia and the Far East (60–65°N). Compared to the methane wetland emissions reported in literature, the wildfire emissions in the south add about 5–20% to their estimated average annual values and are compared with the magnitudes of their interannual variability. Average seasonal cycle peaks in April–May and July–August, which partially overlaps the summertime peak in wetland emissions. The independent estimates from version 3 of Global Fire Emissions Database (GFED3) are by 50% higher (compared to this study) for average annual emissions over the decade (which is quite good regarding the uncertainties) and showed larger differences for individual years. Possible applications of the results are considered for climate research and inverse modelling studies, as well as for assessment of the uncertainties in the present-day wildfire emission estimates.

14/01517 Preparation of a novel PEG composite with halogen-free flame retardant supporting matrix for thermal energy storage application

Qian, Y. *et al. Applied Energy*, 2013, 106, 321–327.
Poly(ethylene glycol) (PEG)/silsesquioxane composite was prepared by *in situ* sol–gel process. The structure of composite was characterized by solid state ^{31}P and ^{29}Si nuclear magnetic resonance and Fourier transform infrared spectroscopy. N_2 adsorption–desorption measurement was used to investigate the porous structure of supporting matrix. Thermal and flame retardancy properties were investigated by differential scanning calorimetry, thermogravimetric analysis and pyrolysis combustion flow calorimetry. Results indicated the PEG composite showed large latent heat (124.7 kJ/kg). After thermal cycling for 1000 cycles, the composite still had large latent heat of 124.1 kJ/kg, showing the composite had good thermal reliability property. The composite had obvious increased intrinsic thermal stability through analysis of integral procedural decomposition temperature. The peak of heat release rate (PHRR) of composite was decreased by 38.6% compared with pure PEG. And the time to PHRR was increased by 31 s compared with pure PEG. The novel shape-stabilized PEG composite had potential to become halogen-free fire resistance phase change composite for thermal energy storage application.

09 PROCESS HEATING, POWER AND INCINERATION

Energy applications in industry

14/01518 A survey of cogeneration in the Italian pulp and paper sector

Comodi, G. *et al. Applied Thermal Engineering*, 2013, 54, (1), 336–344.
The pulp and paper industry is an energy-intensive sector which the need for heat and electricity throughout the year makes an ideal user of cogeneration. This paper presents a survey of cogeneration plants installed in the Italian pulp and paper industry from 1986 to 2010 including the technologies installed and the size and the timeline of installations. The work, carried out in cooperation with ASSOCARTA (the trade organization of Italian pulp, paper and board manufacturers), examines 61 cogeneration plants, 14 of them in detail. The analysis involves 673.5 MWe of installed electrical power, accounting for 75.7% of the sector (890 MWe); the average plant size in the sample is 11.1 MWe, the Italian sector average being 18.2 MWe. Gas turbines coupled with heat recovery steam generators are the commonest technology in the low power range, with 35 plants found between 1 and 8 MWe. If combined cycles (commonly installed above 8 MWe) are considered, the cogeneration plants using gas turbines are 55/61. The data show that from 1986 to 2010 nearly all plants worked with a positive primary energy saving (PES) index, using less primary energy compared to separate production of electrical and thermal energy. Only two plants had a slightly negative PES index, but the price of electricity and natural gas was such that they made a profit anyway.

14/01519 An analysis of energy-related greenhouse gas emissions in the Chinese iron and steel industry

Tian, Y. *et al. Energy Policy*, 2013, 56, 352–361.
With China's increasing pressures on reducing greenhouse gas (GHG) emission, Chinese iron and steel industry (ISI) is facing a great challenge. This study addresses the energy-related GHG emission trajectories, features, and driving forces in Chinese ISI for 2001–2010. First, an energy-related GHG inventory for ISI was made for both scope 1 (direct emissions) and scope 2 (including imported electricity emission). Then, the driving forces for such emission changes were explored by using the method of logarithmic mean Divisa index decomposition analysis. The results indicate that Chinese ISI experienced a rapid growth of energy related GHG emission at average

annual growth rate of 70 million tons CO_2e. Production scale effect was the main driving factor for energy-related GHG emission increase in Chinese ISI, while energy intensity effect and emission factor change effect offset the total increase and energy structure has marginal effect. Construction, manufacture of general purpose and special purpose machinery and manufacture of transport equipment sectors are main sectors for embodied emissions, amounting for more than 75% of the total embodied emissions from Chinese ISI. Such research findings propose that a detailed consideration can help make appropriate polices for mitigating ISI's energy-related GHG emissions.

14/01520 An assessment of a pulp and paper mill through energy and exergy analyses

Utlu, Z. and Kincay, O. *Energy*, 2013, 57, 565–573.

In this study, a pulp and paper mill (PPM) in the SEKA Papermaking Plant in Izmit, Turkey, is analysed through energy and exergy balances. The plant uses recycled wastepaper for papermaking. This type of raw material input makes the process highly sophisticated. The pulping uses strictly mechanical processes, such as digestion, separation by screening and hydrocyclone, and refining. The milling, as an integrated process, provides the final operations necessary to prepare the conditions required for the end-product by stock-preparation, wiring, rolling, and drying by dewatering, pressing and evaporation. The possibility of making the entire process more thermodynamically efficient is discussed by calculating the energy and exergy losses for all the mechanical and physical sub-processes. The study shows that the energy efficiencies for each of the mechanical and physical steps in the PPM vary between 34% and 97.4%, whereas the exergy efficiencies vary between 30.2% and 94.2%. In conclusion, based on the results from the energy and exergy flow analyses, the exergy output can be improved through more efforts directed primarily to further measurements toward more efficient energy use in the PPM.

14/01521 Bio-synthetic natural gas as fuel in steel industry reheating furnaces – a case study of economic performance and effects on global CO_2 emissions

Johansson, M. T. *Energy*, 2013, 57, 699–708.

Climate change is of great concern for society today. Manufacturing industries and construction account for approximately 20% of global CO_2 emissions and, consequently, it is important that this sector investigate options to reduce its CO_2 emissions. One option could be to substitute fossil fuels with renewable alternatives. This paper describes a case study in which four future energy market scenarios predicting 2030 were used to analyse whether it would be profitable for a steel plant to produce bio-synthetic natural gas (bio-SNG) in a biomass gasifier and to substitute liquefied petroleum gas (LPG) with bio-SNG as fuel in reheating furnaces. The effects on global CO_2 emissions were analysed from a perspective in which biomass is considered a limited resource. The results from the analysis show that investment in a biomass gasifier and fuel conversion would not be profitable in any of the scenarios. Depending on the scenario, the production cost for bio-SNG ranged between €22 and €36/GJ. Fuel substitution would reduce global CO_2 emission if the marginal biomass user is a producer of transportation fuel. However, if the marginal user of biomass is a coal power plant with wood co-firing, the result would be increased global CO_2 emissions.

14/01522 Bottoming organic Rankine cycle for a small scale gas turbine: a comparison of different solutions

Clemente, S. *et al. Applied Energy*, 2013, 106, 355–364.

There have been recent efforts devoted to improving the thermal efficiency of small gas turbines in order to approach the typical values of the internal combustion engine at the same range of power. One possibility is represented by a combined cycle, obtained coupling the gas turbine to a bottoming organic Rankine cycle (ORC). This paper deals with the definition of the main features of an ORC system aimed to recover heat from a 100 kWe commercial gas turbine with internal recuperator. After the optimization of the thermodynamic cycles, involving a comparison between six working fluids, different expanders are analysed, with the aim of detecting, if possible, the best-suited machine. First, single stage turbines, in both radial and axial flow configuration, are designed specifically for each considered fluid, in particular investigating the opportunity of mounting the ORC expander directly on the high-speed shaft of the gas turbine. Then, the performances of these dynamic machines are compared with those of positive displacement expanders, such as scroll devices, obtainable from commercial HVAC compressor with minor revisions, and reciprocating ones, here newly designed.

14/01523 Economic and environmental impacts of the energy source for the utility production system in the HDA process

Ouattara, A. *et al. Energy Conversion and Management*, 2013, 74, 129–139.

The well-known benchmark process for hydrodealkylation of toluene (HDA) to produce benzene is revisited in a multi-objective approach for identifying environmentally friendly and cost-effective operation solutions. The paper begins with the presentation of the numerical tools used in this work, i.e. a multi-objective genetic algorithm and a multiple choice decision making procedure. Then, two studies related to the energy source involved in the utility production system (UPS), either fuel oil or natural gas, of the HDA process are carried out. In each case, a multi-objective optimization problem based on the minimization of the total annual cost of the process and of five environmental burdens, that are global warming potential, acidification potential, photochemical ozone creation potential, human toxicity potential and eutrophication potential, is solved and the best solution is identified by use of multiple choice decision making procedures. An assessment of the respective contribution of the HDA process and the UPS towards environmental impacts on the one hand, and of the environmental impacts generated by the main equipment items of the HDA process on the other hand is then performed to compare both solutions. This 'gate-to-gate' environmental study is then enlarged by implementing a 'cradle-to-gate' life cycle assessment, for accounting of emission inventory and extraction. The use of a natural gas turbine, less economically efficient, turns out to be a more attractive alternative to meet the societal expectations concerning environment preservation and sustainable development.

14/01524 Emissions characterization and regulatory compliance at an industrial complex: an integrated MM5/CALPUFF approach

Ghannam, K. and El-Fadel, M. *Atmospheric Environment*, 2013, 69, 156–169.

This paper couples the meteorological mesoscale model (MM5) with the non-steady state CALPUFF modelling system in a short-range dispersion context to assess regulatory compliance with air quality standards in a coastal urban area with complex terrain. For this purpose, an inventory of CO, NO_x and PM_{10} emissions from an industrial complex, highway and quarrying activity was developed using emission factors reported by the US Environmental Protection Agency (USEPA) and the European Environment Agency (EEA). Multiple emission scenarios were then simulated to test the representativeness of the obtained emission factors using statistical analysis of predictions against year-round field measurements. At the validated emission rates, CALPUFF simulations showed an acceptable ability to predict the upper end of observed concentrations and reproduced field measurements at several locations. Statistical analysis revealed that sources are likely to be emitting at conservative estimates (worst-case efficiency of control equipment and fuel quality), with total CO, NO_x and PM_{10} emissions reaching 913 g s^{-1} (19% by highway and 81% by industries), 1266 g s^{-1} (63% by highway and 37% by industries) and 2970 g s^{-1} (93% by industries and 7% by quarries), respectively.

14/01525 Energy efficiency improvement and CO_2 emission reduction opportunities in the cement industry in China

Hasanbeigi, A. *et al. Energy Policy*, 2013, 57, 287–297.

China's annual cement production (i.e. 1868 Mt) in 2010 accounted for nearly half of the world's annual cement production in the same year. This study identified and analysed 23 energy efficiency technologies and measures applicable to the processes in China's cement industry. The conservation supply curve (CSC) used in this study is an analytical tool that captures both the engineering and the economic perspectives of energy conservation. Using bottom–up CSC models, the cumulative cost-effective and technical electricity and fuel savings, as well as the CO_2 emission reduction potentials for the Chinese cement industry for 2010–2030 are estimated. By comparison, the total final energy saving achieved by the implementation of these 23 efficiency measures in the Chinese cement industry over 20 years (2010–2030) is equal to 30% of the total primary energy supply of Latin America or Middle East or around 71% of primary energy supply of Brazil in 2007. In addition, a sensitivity analysis with respect to the discount rate is conducted to assess its effect on the results. The result of this study gives a comprehensive and easy to understand perspective to the Chinese cement industry and policy makers about the energy efficiency potential and its associated cost.

14/01526 Game theory approach in decisional process of energy management for industrial sector

Aplak, H. S. and Sogut, M. Z. *Energy Conversion and Management*, 2013, 74, 70–80.

Intensive energy consuming industrial sectors are the most important actors on global climate change which the natural habitat and the environment face. In this study, by the scope of energy management, decision-making process of the industry and the environment are evaluated in a game theoretic approach. Industry and environment are considered as two players which have conflicting objectives and try to find optimal strategies in governing energy policy. According to concept of study, while industry tries to maintain the sustainability of

production with the strategies of fossil fuel, renewable energies, energy recovery and nuclear energy usage, environment exhibits reactive approach to ensure its sustainability. In the flow of study, players' strategies are analysed by using multi-criteria decision-making methods and by calculating performance efficiency values of strategies, game payoff matrix is obtained. Finally, optimal strategies are found for both industry and environment in orienting their energy policy and results are evaluated. According to results of the payoff matrix, the equilibrium point is the cell (2, 1) with the values of 0.5324 and 0.5619. This implies that the environment develops protective reflexes for sustainable nature in case of using renewable energy in industry.

14/01527 Gas emissions from a large scale circulating fluidized bed boilers burning lignite and biomass

Krzywanski, J. *et al. Fuel Processing Technology*, 2013, 116, 27–34.

A previously established and validated coal combustion model in a circulating fluidized bed (CFB) was used to predict the co-combustion of lignite and biomass processes. The validity of the model was successfully performed on a large-scale 261 MW_e COMPACT CFB boiler. Forest biomass, sunflower husk, willow and lignite coal were applied in co-combustion tests with different shares of biomass and lignite. The energy fraction of biomass in fuel blend was: 7%, 10% and 15%. Emissions of CO_2, CO, SO_2 and NO_x (i.e. $NO + NO_2$) from the co-combustion tests, measured during experiments and predicted by model were compared. The gaseous pollutant emissions, evaluated using the developed model were in a good agreement with experimental results.

14/01528 Investigation of selective catalytic reduction for control of nitrogen oxides in full-scale dairy energy production

Camarillo, M. K. *et al. Applied Energy*, 2013, 106, 328–336.

Selective catalytic reduction (SCR) was used to reduce exhaust gas nitrogen oxides (NO_x) from the emissions of a 710 kW combined heat and power system fuelled by dairy biogas. Exhaust gas NO_x was reduced from 63.1 ± 31.9 to 14.2 ± 17.5 ppmvd @ 15% O_2 such that emissions were 0.33 ± 0.40 g kW^{-1} h^{-1}, based on data averaged over 15 min intervals. Online exhaust gas sensors with integrated process control algorithms were effective in improving NO_x removal by automated control of urea, the ammonia source used for catalysis of NO_x reduction reactions. Pre-SCR NO_x was most strongly correlated with equivalence ratio ($R^2 = 0.39$), indicative of the air–fuel ratio. A concave relationship between NO_x production and thermal conversion efficiency was not observed since lean-burn operation of the engine was consistent and only altered under low engine load. Following installation of pre- and post-SCR NO_x sensors, average daily exhaust gas NO_x reduction in the SCR was 82.6 ± 8.5%. Post-SCR NO_x emissions were typically impacted by pre-SCR NO_x ($R^2 = 0.36$), suggesting that altered operation of the anaerobic digesters or modifications to the engine would be effective in reducing NO_x emissions as well as urea demand. After nearly three years of operation, the SCR catalyst remains in service without requiring replacement. Average daily urea demand was 31.8 ± 16.3 L d^{-1} for the system that produced 369 ± 136 kW of electricity. During the second year of observation the regulatory limit of 0.804 g kW^{-1} h^{-1} was met 94% of the time while the regulatory target of 0.201 g kW^{-1} h^{-1} was only met 45% of the time, based on data averaged over 15 min intervals. These results provide guidance for dairy energy projects in locations with stringent NO_x emissions standards.

14/01529 Investigation of the potential of thermophotovoltaic heat recovery for the Turkish industrial sector

Utlu, Z. and Parali, U. *Energy Conversion and Management*, 2013, 74, 308–322.

Thermophotovoltaics (TPV) are the use of the photovoltaic effect to generate electricity from a high-temperature thermal (infrared) source. This study deals with to provide an overview of heat recovery by TPV from industrial high-temperature processes in Turkish industrial sector. The paper reviews the relevant facts about TPV technology and the high-temperature industry and identifies three principle locations for TPV heat recovery. For each location, one example process is assessed in terms of applicability of TPV impact on the existing process and power scale. Knowledge of these factors should contribute to the design of an optimum TPV system. In the Turkish industrial sector, the total technical–potential energy recovery in the high-temperature industry using deployed and demonstrated heat recovery devices for product, flue gas, and wall heat recovery was estimated as 447.8 PJ/year. However, an estimation of 22.40–67.45 PJ/year can be achieved according to the TPV efficiencies. The paper estimates the range of possible energy savings and the reduction in carbon monoxide emissions using TPV in the high-temperature industry.

14/01530 Modeling and co-simulation of a parabolic trough solar plant for industrial process heat

Silva, R. *et al. Applied Energy*, 2013, 106, 287–300.

In this study, a tri-dimensional non-linear dynamic thermohydraulic model of a parabolic trough collector was developed in the high-level acausal object-oriented language Modelica and coupled to a solar industrial process heat plant modelled in TRNSYS. The integration is performed in an innovative co-simulation environment based on the TLK interconnect software connector middleware. A discrete Monte Carlo ray-tracing model was developed in SolTrace to compute the solar radiation heterogeneous local concentration ratio in the parabolic trough collector absorber outer surface. The obtained results show that the efficiency predicted by the model agrees well with experimental data with a root mean square error of 1.2%. The dynamic performance was validated with experimental data from the Acurex solar field, located at the Plataforma Solar de Almeria, south-east Spain, and presents a good agreement. An optimization of the IST collector mass flow rate was performed based on the minimization of an energy loss cost function showing an optimal mass flow rate of 0.22 kg/s m^2. A parametric analysis showed the influence on collector efficiency of several design properties, such as the absorber emittance and absorptance. Different parabolic trough solar field model structures were compared showing that, from a thermal point of view, the one-dimensional model performs close to the bi-dimensional. Co-simulations conducted on a reference industrial process heat scenario on a South European climate show an annual solar fraction of 67% for a solar plant consisting on a solar field of 1000 m^2, with thermal energy storage, coupled to a continuous industrial thermal demand of 100 kW.

14/01531 Modeling, analysis, and modifications of different GT cooling techniques for modern commercial combined cycle power plants with reducing the irreversibility of the HRSG

Bassily, A. M. *Applied Thermal Engineering*, 2013, 53, (1), 131–146.

The development of efficient techniques of gas turbine (GT) blade cooling has increased the turbine inlet temperature (TIT) significantly. The mass flow rates of GT cooling fluids increase with increasing TIT and the required flow rate of the cooling steam may exceed the available flow rate as TIT increases beyond 1500 °C for the M501H GT combined cycle, mandating the development of a different GT cooling technique that uses less steam for GT blade cooling. Such a cooling technique (steam/air–air GT cooling) applies steam cooling for the first two stages of turbine blade rings (the stationary components only) and was introduced in the development of the M501J GT combined cycle, developed by Mitsubishi Heavy Industries. In this paper, the steam-cooled combustor and the expansions in the gas turbines that utilize the cooling techniques for modern commercial combined cycle power plants (107H/109H GT, M501H GT and M501J GT) are presented, modelled, and analysed. Modifications that enable the M501H GT combined cycle to be operated using the same cooling technique (steam–steam–air GT cooling) at any given TIT and pressure ratio (r_{com}) are presented. Techniques to reduce the irreversibility of the heat recovery steam generator (HRSG) are introduced, leading to significant improvements in both efficiency and power for all cycles.

14/01532 Numerical investigation of oxy-natural-gas combustion in a semi-industrial furnace: validation of CFD sub-models

Galletti, C. *et al. Fuel*, 2013, 109, 445–460.

The modelling through computational fluid dynamics of oxy-natural-gas combustion experimental tests in a 3 MW semi-industrial furnace equipped with a low NO_x burner is discussed. Since the complex geometry of the burner and the size of the furnace, a modelling strategy has been adopted to diminish the computational time and thus to make the simulations affordable. The model aims at validating different sub-models (e.g. combustion/kinetics, radiation/spectral) for oxy-natural-gas fired conditions through the comparison of predictions and in-flame measurements of temperature and chemical species. It is found that fast chemistry approaches are unable to predict the temperature field. The spectral model was also found to play a fundamental role for the correct analysis of such scale devices. Uncertainties in experimental and modelling results are discussed and compared.

14/01533 Opportunities and barriers for efficient energy use in a medium-sized brewery

Sturm, B. *et al. Applied Thermal Engineering*, 2013, 53, (2), 397–404.

Since the 1970s, prices for fuel and raw materials have risen steadily. This change has put the brewing industry under pressure to reduce production costs by intensifying their production process. Additionally, in recent years environmental concerns over greenhouse gas emissions and climate change have arisen among consumers and legislative requirements are getting stricter. Because of these developments, small- and medium-sized breweries are increasingly forced to apply strategies for economic, environmental and social sustainability. This paper gives an overview over the state of the art in the brewing industry

commonly realized in large breweries and presents important barriers to efficiency in smaller companies. The production process of a typical medium-sized brewery in the UK was analysed to identify principal measures to reduce energy and water demands. The case study also examined the particular problems preventing the brewery from realizing these measures. The analysis of the process shows that even basic and easily applicable efficiency measures have so far been neglected. Improving insulation and implementation of basic heat recovery measures could potentially reduce energy demand by 20% and would result in a payback period of 1.3 years.

14/01534 Opportunities for low-grade heat recovery in the UK food processing industry
Law, R. *et al. Applied Thermal Engineering*, 2013, 53, (2), 188–196.
Energy efficiency in the process industry is becoming an increasingly important issue due to the rising costs of both electricity and fossil fuel resources, as well as the tough targets for the reduction in greenhouse gas emissions outlined in the Climate Change Act 2008. Using waste heat sources is key to improving industrial energy efficiency, with an estimated 11.4 TWh of recoverable heat being wasted each year, a quarter of which is from the food and drink processing sector. This paper examines the low-grade waste heat sources common to the food and drink processing sector and the various opportunities for the use of this heat. A review of the best available technologies for recovery of waste heat is provided, ranging from heat transfer between source and sink, to novel technologies for the generation of electricity and refrigeration. Generally, the most economic option for waste heat recovery is heat exchange between nearby/same process source and sink, with a number of well-developed heat exchangers widely available for purchase. More novel options, such as the use of organic Rankine cycles for electricity generation prove to be less economical due to high capital outlays. However, with additional funding provision for demonstration of such projects and development of modular units, such technologies would become more common.

14/01535 Process integration. Tests and application of different tools on an integrated steelmaking site
Grip, C.-E. *et al. Applied Thermal Engineering*, 2013, 53, (2), 366–372.
The energy network in Luleå consists of the steel plant, heat and power production and district heating. Global system studies are necessary to avoid sub-optimization and to deliver energy and/or material efficiency. SSAB began work with global simulation models in 1978. After that several more specialized process integration tools have been tested and used: mathematical programming using a mixed integer linear programming method, exergy analysis and pinch analysis. Experiences and examples of results with the different methods are given and discussed. Mathematical programming has been useful to study problems involving the total system with streams of different types of energy and material and reaction between them. Exergy is useful to describe energy problems involving different types of energy, e.g. systematic analysis of rest energies. Pinch analysis has been used especially on local systems with streams of heat energy and heat exchange between them.

14/01536 The effect of substrate and operational parameters on the abundance of sulphate-reducing bacteria in industrial anaerobic biogas digesters
Moestedt, J. *et al. Bioresource Technology*, 2013, 132, 327–332.
This study evaluated the effects of operational parameters and type of substrate on the abundance of sulfate-reducing bacteria in 25 industrial biogas digesters using qPCR targeting the functional dissimilatory sulfite reductase gene. The aim was to find clues for operational strategies minimizing the production of H_2S. The results showed that the operation, considering strategies evaluated, only had scarce effect on the abundance, varying between 10^5 and 10^7 gene copies per ml. However, high ammonia levels and increasing concentration of sulfate resulted in significantly lower and higher levels of sulfate-reducing bacteria, respectively.

14/01537 Thermal energy management in the bread baking industry using a system modelling approach
Paton, J. *et al. Applied Thermal Engineering*, 2013, 53, (2), 340–347.
Energy usage in bread ovens is analysed using a generic methodology applicable to all types of mass-production tunnel ovens. The presented methodology quantifies the energy required to bake the dough, and to conduct a detailed analysis of the breakdown of losses from the oven. In addition, a computational fluid dynamics (CFD) optimization study is undertaken, resulting in improved operating conditions for bread baking with reduced energy usage and baking time. Overall, by combining the two approaches, the analyses suggest that bake time can be reduced by up to 10% and the specific energy required to bake each loaf by approximately 2%. For UK industry, these savings equate to more than £0.5 million cost and carbon reduction of more than 5000 tonnes CO_2 per year.

14/01538 Ultra low sulfur diesel simulation. Application to commercial units
Paz-Zavala, C. D. L. *et al. Fuel*, 2013, 110, 227–234.
A kinetic model for the hydrodesulfurization process to obtain ultra-low sulfur diesel (ULSD) was applied to commercial units proving its capabilities. The model was developed from the experimental data that were generated in a pilot plant with three commercial catalysts (*A*, *B* and *C*), using straight run gasoil (SGO), light cycle oil (LCO), light cracked gasoil (LCGO) and their blends as feedstocks. The model was compared with operational data of one refinery of Latin America. Typical conditions have been covered by the simulation analysis (340–370 °C, 0.7–1.5 h^{-1} and 60–80 kg/cm^2, for temperature, space velocity and pressure, respectively) in order to obtain model predictions compared to those used in practical industrial applications.

14/01539 Which industry is greener? An empirical study of nine industries in OECD countries
Fujii, H. and Managi, S. *Energy Policy*, 2013, 57, 381–388.
This study analysed the relationship between the CO_2 emissions of different industries and economic growth in developed countries from 1970 to 2005. The authors tested an environmental Kuznets curve (EKC) hypothesis and found that total CO_2 emissions from nine industries show an N-shaped trend instead of an inverted U or monotonic increasing trend with increasing income. The EKC hypothesis for sector-level CO_2 emissions was supported in the (1) paper, pulp, and printing industry; (2) wood and wood products industry and (3) construction industry. The authors also found that emissions from coal and oil increase with economic growth in the steel and construction industries. In addition, the non-metallic minerals, machinery, and transport equipment industries tend to have increased emissions from oil and electricity with economic growth. Finally, the EKC turning point and the relationship between gross domestic product per capita and sectoral CO_2 emissions differ among industries according to the fuel type used. Therefore, environmental policies for CO_2 reduction must consider these differences in industrial characteristics.

10 SPACE HEATING AND COOLING/HEAT PUMPS

14/01540 Effects of continuous sonication on laminar convective heat transfer inside a tube using water–TiO_2 nanofluid
Rayatzadeh, H. R. *et al. Experimental Thermal and Fluid Science*, 2013, 48, 8–14.
In this research, an experimental study is carried out to investigate the effect of adding TiO_2 nanoparticles to the distilled water on convective heat transfer and pressure drop with and without continuous induced ultrasonic field in the nanofluid's reservoir under constant heat flux. Experiments are done for laminar flow regime with volume concentration, up to 0.25%. It is observed that adding nanoparticles to the base liquid enhances Nusselt number, and more particle concentration leads to more enhancements in Nusselt number except for 0.25% volume concentration. Results also show that the Nusselt number of the nanofluids at the volume concentration of 0.25 vol.% was approximately the same as base fluids for the given conditions. In addition, the achievements demonstrate that inducing ultrasonic field increases Nusselt numbers dramatically compared with those results obtained with no sonication. Finally, no significant increase occurs in pressure drop in the range of studied volume fractions.

14/01541 A comprehensive experimental analysis of gadolinium active magnetic regenerators
Tušek, J. *et al. Applied Thermal Engineering*, 2013, 53, (1), 57–66.
The main goal of this study was an experimental comparison of six different active magnetic regenerators (AMRs) with gadolinium as the magnetocaloric material. The analysis was carried out for three different parallel-plate AMRs (with different porosities and different orientations of the plates in the magnetic field) and three different packed-bed AMRs (filled with spheres, powders and cylinders). Since the operation of an AMR is strongly affected by the operating conditions, the experiments were performed at different mass-flow rates and at different operating frequencies. These were required in order to define the optimum corresponding operating conditions for the analysed AMRs. As comparative criteria the maximum temperature span, the cooling capacity and the experimentally predicted *COP* were taken into consideration. The experimental analysis was performed on a new prototype of magnetic refrigerator designed as an experimental device. Its operation is based on the linear movement of a permanent-magnet assembly over a static AMR. The magnet assembly provides a measured magnetic field of about 1.15 T. The

results reveal that the geometry of the AMR (the form of the magnetocaloric material) has a crucial impact on the performance of the magnetic refrigerator. The best overall cooling characteristics (temperature span, cooling capacity and *COP*) were obtained for the parallel-plate AMR with the smallest porosity (~25%) and the orientation of the plates parallel to the magnetic field. This particular AMR generated a temperature span of 20 K, which is also the largest, so-far measured and published temperature span with a parallel-plate AMR for a given magnetic field change generated by permanent magnets. With respect to the comparison of the experimentally predicted *COP* values, the parallel-plate AMRs show higher efficiencies than the packed-bed AMRs.

14/01542 A graphite nanoplatelet/epoxy composite with high dielectric constant and high thermal conductivity

Min, C. *et al. Carbon*, 2013, 55, 116–125.

A simple strategy for the preparation of composites with high dielectric constant and thermal conductivity was developed through a typical interface design. Graphite nanoplatelets (GNPs) with a thickness of 20–50 nm are fabricated and homogeneously dispersed in the epoxy matrix. A high dielectric constant of more than 230 and a high thermal conductivity of 0.54 W/mK (a 157% increase over that of pure epoxy) could be obtained for the composites with a lower filler content of 1.892 vol.%. The dielectric constant still remains at more than 100 even in the frequency range of 10^5–10^6 Hz. When loaded at 2.703 vol.%, GNP/epoxy composites have a dielectric constant higher than 140 in the frequency range of 10^2–10^4 Hz and a high thermal conductivity of 0.72 W/mK, which is a 240% increase over that of pure epoxy. The high dielectric constant and low loss tangent are observed in the composite with the GNPs content of 0.949 vol.% around 10^4 Hz. It is believed that high aspect ratio of GNPs and oxygen functional groups on their basal planes are critical issues of the constitution of a special interface region between the GNPs and epoxy matrix and the high performance of the composites.

14/01543 A multi-criteria decision analysis based assessment of walling materials in India

Sabapathy, A. and Maithel, S. *Building and Environment*, 2013, 64, 107–117.

Building construction in India is estimated to grow at a rate of 6.6% per year between 2005 and 2030 resulting in a continuous increase in demand for building materials. Fired clay bricks are the most widely used walling materials in the country. However, over the past few decades, the development of other materials such as concrete blocks, fly ash bricks, stabilized mud blocks, etc., has created viable alternatives to bricks. There is limited understanding of the broader environmental consequences of these building materials addressing natural resource depletion, energy, environment and socio-economic impacts. The main objective of this paper is to present a comprehensive assessment of materials used for wall construction by comparing one square meter of constructed wall for each of the materials. A composite environmental index was developed by weighting and aggregating normalized numerical scores of several parameters making use of a multi-criteria decision analysis framework. The environmental index was then ranked to determine walling systems that are best suited in the context of India. This analysis shows that wall assemblies that use non-fired products as masonry units are ranked higher compared to fired masonry unit wall assemblies. Clay fired masonry wall assemblies exhibit poorer environmental performance compared to non-fired masonry wall assemblies. When a more efficient form of construction such as the Rat-trap bond wall construction is considered, the environmental performance of clay fired brick walls is significantly improved.

14/01544 A novel optimization approach of improving energy recovery in retrofitting heat exchanger network with exchanger details

Pan, M. *et al. Energy*, 2013, 57, 188–200.

Improving energy recovery with retrofitting heat exchanger network (HEN) has been widely studied in academic and industrial communities. Distinct from most of existing works on HEN retrofit neglecting exchanger geometry, this paper presents a novel optimization method for dealing with the main exchanger geometry details in HEN retrofit problems. The addressed details of shell and tube exchangers include tube passes, shell passes, heat transfer intensification, logarithmic mean temperature difference (LMTD), and LMTD correction factor (FT), which are systematically identified under given objective function and topological constraints in the existing heat recovery systems. Based on the recent works on HEN retrofit scenarios addressing network topology modification, an efficient optimization framework, consisting of two optimization stages with the implementation of mixed integer linear programming-based iterative method, has been developed to deal with the computational difficulties associated with the non-linearity of LMTD and FT. Case study from literature examples are carried out to demonstrate the validity and soundness of the proposed approach, showing that the new proposed approach is able to provide realistic and practical solutions for debottlenecking of HEN with systematic consideration of exchanger details.

14/01545 A three-dimensional two-phase flow model with phase change inside a tube of petrochemical pre-heaters

Fontoura, D. V. R. *et al. Fuel*, 2013, 110, 196–203.

The transport of fluids in industrial units takes place usually inside cylindrical ducts. Multiphase systems flowing inside pipes are very common and many times there are also mass, energy and momentum transfer. Two-phase flow is found in many petrochemical processes, as is the case of preheating furnaces where normally the liquid vaporizes as it flows inside the heater. In the great majority of these heaters, there is a phase change from liquid to gas. The objective of this work is to simulate the two-phase gas–liquid flow of crude oil inside pipes of petrochemical fired heaters with the use of a computational fluid dynamics (CFD) model to be later used in the prediction of coke formation through a thermal cracking model and a ternary solubility diagram for the petrol feed. The CFD free software OpenFOAM was used. There is a growing interest in the use of the OpenFoam project and many successful models have been implemented using this software. New routines were implemented to estimate temperature and concentration inside the tube, taking into consideration the interaction between the phases. To estimate the momentum it was used a phase intensive formulation for dispersed two-phase flow already implemented in OpenFOAM. The temperature profiles were predicted. The *k*-epsilon model was used to describe the turbulence and a vaporization model was implemented to estimate the phase change. A kinetic reaction net for crude oil with seven lumps was used in order to predict the thermal cracking of the crude oil.

14/01546 Assessment of a new model for the linear and nonlinear stability analysis of natural circulation loops with supercritical fluids

Debrah, S. K. *et al. Annals of Nuclear Energy*, 2013, 58, 272–285.

The paper describes the characteristics and the first applications of models recently developed to analyse both transient and linear stability of natural circulation loops, also accounting for the presence of heat structures. The models were conceived to be applied to loops containing fluids at supercritical pressure, though in principle they can be applied to a variety of fluids, even in usual single-phase and two-phase conditions. With respect to available system codes and already published models, the advantage of the twin programmes set up in this work is to make use exactly of the same numerically discretized equations for transient and linear stability analyses, giving a clearer perspective of the obtained results, also including the effect of heat structures. For purpose of assessing the new models, a systematic comparison with the results obtained by the RELAP5 code results is performed, showing a very high level of coherence in very different conditions, including or not heat structures. The models are then applied to an experiment already addressed in previous work, better justifying the obtained conclusions.

14/01547 Characterization of panels containing micro-encapsulated phase change materials

Marchi, S. *et al. Energy Conversion and Management*, 2013, 74, 261–268.

A solution to increase passively the thermal inertia of lightweight wallboard for building envelopes is to incorporate a phase change material (PCM). The thermal mass and thermal conductivity of the panels establish the thermal inertia of the envelope, which causes a damping and time lag of the temperature peaks inside the buildings. The knowledge of the thermal properties of the wallboard is the base of the modelling of buildings, a target uncertainty can be calculated from the modelling purposes. This paper is devoted to the characterization of a panel containing PCM for its thermal properties. Particular attention is devoted to the calculation of the uncertainty of the thermal properties. Commercial microencapsulated paraffin-based PCMs and specific binders have been used to prepare panels. PCMs have been characterized by granulometric and thermogravimetric analysis and the porosity of each panel has been determined experimentally by mercury porosimetry. The microstructure of the panels has been observed by scanning electron microscope analysis in order to recognize the nature of the porous structure. The theoretical effective thermal conductivity of the PCM embedded in the polyurethane resin has been predicted by different models; especially the Maxwell–Eucken and the effective medium theory (EMT) equations just on the basis of the volume fractions and the thermal conductivities of the components. The thermal conductivity estimated with the EMT model closely followed the experimental data measured by thermofluximeter method and the accuracy of the prediction has been analysed evaluating the uncertainty budget with respect to all the variables of the model. The accuracy of the method resulted to be acceptable for modelling the thermal performance of a building.

14/01548 Comparative study on the thermal reactivation of spent adsorbents

Román, S. *et al. Fuel Processing Technology*, 2013, 116, 358–365.

Activated carbons previously used for p-nitrophenol (PNP) adsorption were subjected to thermal reactivation in order to recover their initial porosity characteristics. Three activating agents were comparatively analysed (air, carbon dioxide and water steam). Regeneration results improved in the sequence air < CO_2 < steam; steam activation almost removed all the adsorbate adsorbed on the carbon, achieving regeneration efficiency values up to 94% for N_2 adsorption, and above 100% for PNP adsorption. The activation process did not cause a significant modification of the pore size distribution of the adsorbents, which remained microporous irrespective of the activating agent. The analysis of gases evolved was consistent with the chemical processes involved in the respective activations. There was a significant difference in the pattern followed by H_2 in steam activations compared with CO_2 and air. The prominence of water gas and water gas shift reactions were associated to this effect, which was also evident from the increase in CO and CO_2 concentration.

14/01549 Composite macrocapsule of phase change materials/expanded graphite for thermal energy storage

Li, W. *et al. Energy*, 2013, 57, 607–614.

Three kinds of macro-encapsulated phase change materials (Macro-PCMs) were fabricated, i.e. MacroPCMs with a single core–shell structure, MacroPCMs containing microencapsulated phase change materials (MicroPCMs), and composite macrocapsules of MicroPCMs/expanded graphite prepared by suspension-like polymerization followed by a piercing–solidifying incuber process. The morphology, microstructure, phase change property, as well as seal tightness were systematically characterized by field emission scanning electron microscope, differential scanning calorimetry, and energy dispersive X-ray spectrometer. The core–shell structured macrocapsules exhibit a homogeneous thickness shell. The interface combination between MicroPCMs and polymer substrate was studied through the cross section micrograph of MacroPCMs containing MicroPCMs. The morphology and seal tightness of MacroPCMs fabricated with expanded graphite absorbing both PCMs and shell-forming monomers, enhanced significantly compared with that of PCMs alone. In addition, the effects of polymer substrate proportion between styrene-maleic anhydride copolymer and sodium alginate on the microstructure and performance of MacroPCMs were discussed as well.

14/01550 Coupled TRNSYS-CFD simulations evaluating the performance of PCM plate heat exchangers in an airport terminal building displacement conditioning system

Gowreesunker, B. L. *et al. Building and Environment*, 2013, 65, 132–145.

This paper reports on the energy performance evaluation of a displacement ventilation (DV) system in an airport departure hall, with a conventional DV diffuser and a diffuser retrofitted with a phase change material storage heat exchanger (PCM-HX). A TRNSYS-CFD quasi-dynamic coupled simulation method was employed for the analysis, whereby TRNSYS® simulates the HVAC and PID control system and ANSYS FLUENT® is used to simulate the airflow inside the airport terminal space. The PCM-HX is also simulated in CFD, and is integrated into the overall model as a secondary coupled component in the TRNSYS interface. Different night charging strategies of the PCM-HX were investigated and compared with the conventional DV diffuser. The results show that: (i) the displacement ventilation system is more efficient for cooling than heating a space; (ii) the addition of a PCM-HX system reduces the heating energy requirements during the intermediate and summer periods for specific night charging strategies, whereas winter heating energy remains unaffected; (iii) the PCM-HX reduces cooling energy requirements; and (iv) maximum energy savings of 34% are possible with the deployment of PCM-HX retrofitted DV diffuser.

14/01551 Design and study of an electrical liquid heater using conductive polymer composite tubes

Noel, H. *et al. Applied Thermal Engineering*, 2013, 54, (2), 507–515.

This study focuses on both the design and testing of an electrical heating device using current passage tubes made of conductive polymer composites (CPC). To obtain such materials, an insulating polymer matrix is combined with electrical conductive fillers (carbon black, carbon fibres or metal particles). Power dissipation is observed when an electrical current is passed through the charged polymer matrix. To optimize the heater design, two different axisymmetric, $T(r,z)$ finite element models were developed with COMSOL®. The first model represents the electro-thermal behaviour of a current passage tube with internal water flow only. The second one takes into account water circulation both inside and outside the heating tube. A prototype was developed based on four immersed CPC tubes supplied electrically and hydraulically in parallel in a PVC casing. The experimental sequences performed on this pilot coupled with a hydraulic circuit made it possible to validate the two models. Analysis of the experimental recordings indicated that thermoelectric efficiency was higher than 90%. The thermal behaviour of such heaters was well defined on the basis of the information obtained from these tests and on the numerical simulations.

14/01552 Dodecanoic acid as a promising phase-change material for thermal energy storage

Desgrosseilliers, L. *et al. Applied Thermal Engineering*, 2013, 53, (1), 37–41.

The melting transition of dodecanoic acid ($CH_3(CH_2)_{10}COOH$, also known as lauric acid) has been examined with a view to use for latent heat energy storage in solar thermal applications. The influence of purity (reagent grade [98% pure] compared with practical grade [<80% pure]) on the melting transition was found to be insignificant. The long-term stability of the melting transition of practical-grade dodecanoic acid was investigated by thermal cycling of samples from completely solid through complete melting and back to the solid phase, nearly 500 times. It was found that the transition enthalpy and the melting onset temperature remain within experimental uncertainty of their values, $184\,J\,g^{-1}$ and 43.3 °C, respectively. Neither data set showed significant trends with number of thermal cycles. The freezing temperature of 41 °C for practical-grade dodecanoic acid also was stable with respect to thermal cycling, showing almost negligible hysteresis, without addition of nucleating agents. The specific heat in the region of the phase transition was determined, along with the thermal conductivity in the solid state ($0.150 \pm 0.004\,W\,m^{-1}\,K^{-1}$ at 30 °C) and the volume change associated with melting (6%). Although the thermal conductivity of dodecanoic acid is low in both the solid phase and liquid phase, and thermal energy storage devices would need to be designed accordingly, dodecanoic acid is inexpensive, readily available (used as a foodstuff), has a low volume change on melting, and is stable over hundreds of thermal cycles even in practical grade, making it a promising phase-change material for thermal energy storage.

14/01553 Effect of longitudinal pitch on convective heat transfer in crossflow over in-line tube banks

Kim, T. *Annals of Nuclear Energy*, 2013, 57, 209–215.

An analytical study using a computational fluid dynamics code has been performed to investigate the effect of the longitudinal pitch on the single-phase heat transfer characteristics in crossflow over in-line tube banks. A simplified geometry with periodic and symmetric boundary conditions is employed for the analysis. A sensitivity analysis using various two-equation turbulence models has been conducted to examine the impact of the turbulence model on the heat transfer characteristics and to determine a turbulence model that can describe the physical phenomena of interest appropriately. The result indicates that the heat transfer coefficient might be reduced by 37.1% from the prediction by a well-known correlation by Zukauskas as the longitudinal pitch decreases. By analysing the result, it is found that the heat transfer degradation can be estimated by using an empirical correction factor and the Zukauskas' correlation can predict existing experimental data when the correlation is combined with the empirical correction factor developed in this study.

14/01554 Effect of U-tube length on reverse flow in UTSG primary side under natural circulation

Hao, J. *et al. Annals of Nuclear Energy*, 2013, 56, 66–70.

For natural circulation, it is shown that parallel flow in the tubes of inverted U-tube steam generators may be non-uniform, and reverse flow occurs within some U-tubes. However the current researches on the mechanism and space distribution of reverse flow in the U-tubes gave different results. In present work, a model of one-dimension and steady state flow is proposed, which can be used to analyse the effect of U-tube length on reverse flow in UTSG primary side under natural circulation. According to the linear micro-disturbance theory, the mechanism of reverse flow is studied. The relationships between U-tube length and critical pressure drop and critical velocity are non-linear, at which the flow instability happens. There exists a critical U-tube length which has the maximal absolute value of critical pressure drop. The results are validated by the best estimate code RELAP5/MOD3.3.

14/01555 Experimental and numerical study of the thermal performance of a new type of phase change material room

Meng, E. *et al. Energy Conversion and Management*, 2013, 74, 386–394.

A new type of phase change material (PCM) room was proposed in this paper to control the indoor air temperature for a better thermal comfort for human beings. That is to place two different kinds of PCM into room envelopes of different orientations. Both experimental and numerical studies were carried out for rooms with/without PCM. Indoor air temperature and interior surface heat flux of the two rooms were studied in typical summer and winter climate of Shanghai (31.2°N, 121.5°E). Important factors that affect the thermal perform-

ance of the PCM were studied, such as phase change temperature, thickness of the PCM and the arrangement of the two kinds of PCM in the room. Results showed that this new type of PCM room can decrease the indoor air temperature fluctuation by 4.3 °C in summer and 14.2 °C in winter. Different arrangements of the two kinds of PCM in the room can cause an indoor air temperature difference to be 6.9 °C in summer and 2.7 °C in winter.

14/01556 Experimental evaluation of sodium to air heat exchanger performance

Vinod, V. *et al. Annals of Nuclear Energy*, 2013, 58, 6–11.

Sodium to air heat exchangers (AHXs) is used in prototype fast breeder reactor (PFBR) circuits to reject the decay heat produced by the radioactive decay of the fission products after reactor shutdown, to the atmospheric air. The heat removal through sodium to air heat exchanger maintains the temperature of reactor components in the pool within safe limits in case of non-availability of normal heat transport path. The performance of sodium to air heat exchanger is very critical to ensure high reliability of the decay heat removal systems in sodium cooled fast breeder reactors. Hence experimental evaluation of the adequacy of the heat transfer capability gives confidence to the designers. A finned tube cross flow sodium to air heat exchanger of 2 MW heat transfer capacity with sodium on tube side and air on shell side was tested in the steam generator test facility at Indira Gandhi Center for Atomic Research, India. Heat transfer experiments were carried out with forced circulation of sodium and air, which confirmed the adequacy of heat removal capacity of the heat exchanger. The testing showed that 2.34 MW of heat power is transferred from sodium to air at nominal flow and temperature conditions. A one dimensional computer code developed for design and analysis of the sodium to air heat exchanger was validated by the experimental data obtained. An equivalent Nusselt number, Nu_{eq} is derived by approximating that the resistance of heat transfer from sodium to air is contributed only by the film resistance of air. The variation of Nu_{eq} with respect to the Reynolds number was studied.

14/01557 Experimental investigation on laminar forced convection heat transfer of ferrofluids under an alternating magnetic field

Ghofrani, A. *et al. Experimental Thermal and Fluid Science*, 2013, 49, 193–200.

This research study presents an experimental investigation on forced convection heat transfer of an aqueous ferrofluid flow passing through a circular copper tube in the presence of an alternating magnetic field. The flow passes through the tube under a uniform heat flux and laminar flow conditions. The primary objective was to intensify the particle migration and disturbance of the boundary layer by utilizing the magnetic field effect on the nanoparticles for more heat transfer enhancement. Complicated convection regimes caused by interactions between magnetic nanoparticles under various conditions were studied. The process of heat transfer was examined with different volume concentrations and under different frequencies of the applied magnetic field in detail. The convective heat transfer coefficient for distilled water and ferrofluid was measured and compared under various conditions. The results showed that applying an alternating magnetic field can enhance the convective heat transfer rate. The effects of magnetic field, volume concentration and Reynolds number on the convective heat transfer coefficient were widely investigated, and the optimum conditions were obtained. Increasing the alternating magnetic field frequency and the volume fraction led to better heat transfer enhancement. The effect of the magnetic field in low Reynolds numbers was higher, and a maximum of 27.6% enhancement in the convection heat transfer was observed.

14/01558 Experimental investigation on the energy performance of Living Walls in a temperate climate

Mazzali, U. *et al. Building and Environment*, 2013, 64, 57–66.

Living walls, a type of vertical greenery system, are relatively light structures for architectural green cladding. They embed a thick curtain of plants nurtured by an automated watering system. Three living wall field tests are presented for investigating potential effects of the energy behaviour on building envelopes. In particular, living walls were monitored in a Mediterranean temperate climate context at the latitudes of northern and central Italy. As a result, the dependence on the solar radiation forcing came out clearly. During sunny days, difference in temperature (monitored on the external surface) between the bare wall and the covered wall ranges from a minimum of 12 °C (case C) to a maximum of 20 °C (case A). The analysis was extended also to heat flux. The incoming (positive) heat flux through the bare wall was found to be higher compared to the living wall. Considering an overall thermal balance during the monitoring period, the outgoing heat flux through the living wall was higher. These results indicate that the use of green architectural cladding can significantly contribute to cooling energy reduction and offer a valuable solution for retrofitting existing buildings.

14/01559 Experimental investigations of flat plate heat pipes with interlaced narrow grooves or channels as capillary structure

Wang, C. *et al. Experimental Thermal and Fluid Science*, 2013, 48, 222–229.

Experimental investigations of two different flat plate heat pipes (FPHPs) are presented. The capillary structure is made of intersected narrow grooves for the first FPHP and interlaced channels for the second FPHP. The copper heat pipes, filled with deionized water, were tested in different heat fluxes and working fluid filling ratios. The temperature fields and overall thermal resistances of the heat pipes under different experimental conditions are studied. The experiments were performed with copper radiator and electronic fan which have been commercially applied for CPU cooling to simulate a practical application. The results indicate that the optimal filling ratios of the FPHPs are 65% for FPHP 1 and 70% for FPHP 2. The smallest thermal resistances of FPHPs at their optimal filling ratios are 0.183 K/W and 0.071 K/W for FPHP 1 and FPHP 2, respectively. The thermal performances of the FPHPs in both axial and radial directions at various heat fluxes are also investigated. The results disclose that the special design of FPHP 2 can improve the heat conduction in axial direction and enhance the capillary effect. Otherwise, the temperature levelling ability of both FPHPs on cooling surface is similar in radial direction.

14/01560 Heat conduction in nuclear fuel by the Kirchhoff transformation

Tomatis, D. *Annals of Nuclear Energy*, 2013, 57, 100–105.

Realistic simulations of nuclear reactors by computer codes are complex multi-physics problems, coupled through different physical feedbacks on nuclear cross sections. Within these calculations, heat conduction in fuel rods has a crucial importance, especially in thermal reactors, providing the fuel temperature necessary to reproduce the Doppler broadening effect. In this work, the Kirchhoff transformation is applied to solve the non-linear heat conduction problem in the classical fuel rod model. Comparisons with the common numerical scheme based on successive substitutions are presented in a simple case, also discussing the higher computational performances achieved by this integral transformation. Moreover, polynomial approximations are introduced to obtain further computational gain. This technique yields almost analytical fuel temperature distributions, thus ensuring high accuracy in the evaluation of the neutron reactivity from the Doppler effect of nuclear fuel.

14/01561 Heat dissipation performance of MWCNTs nano-coolant for vehicle

Teng, T.-P. and Yu, C.-C. *Experimental Thermal and Fluid Science*, 2013, 49, 22–30.

This study demonstrates the heat dissipation performance of a motorcycle radiator filled with multi-walled carbon nanotubes (MWCNTs) nano-coolant (NC). The two-step synthesis method was used to produce different concentrations of MWCNTs/water (W) nanofluid (0.1, 0.2, and 0.4 wt%) using a 0.4 wt% cationic chitosan dispersant, and the MWCNTs/W nanofluid was mixed with ethylene glycol (EG) at a 1 : 1 volume ratio to form the NC_1, NC_2 and NC_3. The experiments in this study measured the thermal conductivity, viscosity and specific heat of NC with weight fractions and sample temperatures (80, 85, 90 and 95 °C), and then used the NC in an air-cooled radiator for a motorcycle to assess its heat exchange capacity, Nusselt number and pumping power under different volumetric flow rates (4.5, 6.5 and 8.5 L/min) and sample temperatures (80, 85, 90 and 95 °C). Considering the overall efficiency of the heat exchange system, this study evaluates the relationship of heat exchange capacity and the pumping power using the efficiency factor (EF). Experimental results show that the NC_1 has a higher heat exchange capacity and EF than EG/W. The maximum enhanced ratios of heat exchange, pumping power, and EF for all the experimental parameters in this study were approximately 12.8%, 4.9% and 14.1%, respectively, compared with EG/W. NC with high concentrations of MWCNTs cannot achieve a better heat exchange capacity because the uneven density of NC in the flow state increases the thermal resistance of the solid–liquid interface, effectively decreasing the contact area between the MWCNTs and the EG/W.

14/01562 Heat transfer enhancement in a tube fitted with helical blade rotors with grooves

Zhang, Z. *et al. Experimental Thermal and Fluid Science*, 2013, 48, 169–176.

Experiments were carried out in order to evaluate the heat transfer and friction characteristics of the circular tube fitted with helical blade rotors with grooves. Meanwhile, the influence of the space between rotors, rotor number in each group and entrance distance on heat transfer, friction factor and thermal performance factor was also investigated. An experiment using a smooth tube was carried out to calibrate the experimental system and data reduction method. The experimental results revealed that the helical blade rotors with grooves

improved heat transfer with the Nusselt number increasing by 17.1–22.4% and friction factor increasing by 16.9–57.4% within the experimental Reynolds number range; meanwhile, the thermal performance factor of the rotors inserted tube was higher than 1.0, which validated the practical heat transfer enhancement function of the rotors. Furthermore, the comparison results of different assembled modes indicated that both the Nusselt number and friction factor increased with the decreasing space between rotors, rotor number in each group and entrance distance; the thermal performance factor improved with the decreasing space between rotors and entrance distance; and five rotors in each group offered a better thermal performance and generated higher heat transfer enhancement than both one rotor in each group and ten rotors in each group.

14/01563 Heat transfer enhancement of NBI vacuum pump cryopanels

Guaman, S. O. *et al. Fusion Engineering and Design*, 2013, 88, (6–8), 882–886.

Huge cryogenic pumps are installed inside neutral beam injectors in order to manage the typically very large gas flows. This paper deals with the aspect of passive cooling in NBI cryopump design development and discusses design considerations in two example areas. One is the design of cryopanels consisting of a pipe, centrally supplied with cryogenic helium, and a welded fin, passively cooled, to provide the necessary pumping surface below a given maximum temperature. The results of several parametric simulations in ANSYS are presented using different copper thicknesses and cryopanel geometries to discuss the thermal capability (heat transfer characteristics and heat capacities) of a number of design variants. The optimum design solution is based on copper-coated fins, using an electroplating technique, and thereby improving the heat transfer of the cryopanels while attaining an overall reduction in weight. The other area is the sound design of the manifold shielding system with a weld contact between copper and stainless steel. Weld samples were manufactured and investigated to raise awareness of the demands and risks during manufacturing and to demonstrate that readily applicable weld procedures exist.

14/01564 Heat transfer in upper part of electrolytic cells: thermal circuit and sensitivity analysis

Zhao, Z. *et al. Applied Thermal Engineering*, 2013, 54, (1), 212–225.

A thermal circuit representation was developed to study the heat transfer mechanisms in the top section of an aluminium smelting pot. In view of thermal management and waste heat recovery applications, the sensitivity of the off-gas temperature and of the heat content in the gas with respect to several parameters was investigated. It was found that the draft condition was the most influential parameter. Additionally, the convection coefficients on the anode cover, and on the yoke and stubs proved to have a stronger influence on exhaust gas temperature, compared with the heat transfer coefficients on the hoods and rod. The results indicate that it is conceptually possible to increase both the gas temperature and the heat content, while maintaining at the same time the current operating conditions of the cell. Variations of the potroom temperature, hood insulation and anode height were also considered and affected significantly the gas temperature.

14/01565 Internal and external fin heat transfer enhancement technique for latent heat thermal energy storage in triplex tube heat exchangers

Al-Abidi, A. A. *et al. Applied Thermal Engineering*, 2013, 53, (1), 147–156.

The importance of latent heat thermal energy storage is significant in contrast to sensible energy storage because of the large storage energy densities per unit mass/volume at nearly constant thermal energy. In this paper, heat transfer enhancement technique by using internal and external fins for phase change material (PCM) melting in a triplex tube heat exchanger (TTHX) was investigated numerically. A two-dimensional numerical model is developed using the Fluent 6.3.26 software program, and pure conduction and natural convection are considered in the simulation. The number of fins, fin length, fin thickness, Stefan number, TTHX material and the PCM unit geometry in the TTHX are found to influence the time for complete melting of the PCM. Experiments were conducted to validate the proposed model. Simulated results agree with the experimental results. The computational results show that case G (eight-cell PCM unit geometry) achieved a shorter time in completing the melting of the PCM, the total melting time is decreased to 34.7%.

14/01566 Modelling of isobaric stages of adsorption cooling cycle: an optimal shape of adsorption isobar

Okunev, B. N. *et al. Applied Thermal Engineering*, 2013, 53, (1), 89–95.

This paper addresses the effect of the adsorption isobar shape on dynamics of the isobaric stages of adsorption chillers which are considered as real alternative to common compression and absorption machines. The authors used a mathematical model of coupled heat and mass transfer in a spherical adsorbent grain that is in thermal contact with a metal plate subjected to a fast temperature jump/drop from 60 to 70 °C. Several model isobars of water adsorption (stepwise, linear and exponential) are tested to elucidate the effect of the isobar shape. Temporal evolution of radial profiles of the temperature, pressure and adsorbed water concentration inside the grain is calculated and analysed. In most cases, the calculated dependencies of the average water uptake/release can be satisfactorily described by an exponential function up to the dimensionless conversions of 0.7–0.8. The characteristic adsorption/desorption time τ is found to be strongly dependent on the isobar shape. Both adsorption and desorption processes are fastest for the step-like isobar, with the step positioned at temperature as much different from the final temperature of the metal plate as possible, because in this case the driving force for adsorption/desorption process is maximal. Appropriate recommendation on enhancing the adsorption chiller dynamics is made.

14/01567 Natural nanofluid-based cooling of a protuberant heat source in a partially-cooled enclosure

Guimarães, P. M. and Menon, G. J. *International Communications in Heat and Mass Transfer*, 2013, 45, 23–31.

This work investigates a two-dimensional natural convection in a square enclosure with a protuberant heat source that may resemble an electrical transformer. It is a laminar and non-steady regime. The finite element method is used to approximate solutions. Linear quadrilateral elements are employed to spatially discretize the domain. Several validations are carried out with numerical and experimental results. Water-based nanofluids have copper or alumina or titanium oxide as their nanoparticles. Lateral vertical cold walls have variable heights and they are referred to fins, which could be considered to be part of the cooling system to refrigerate electrical transformers, for example. Ten heights are studied for these cold walls. Rayleigh number ranges from 10^5 to 10^6 and the volume fraction from 0 to 0.016, totalling nine suspension concentrations. By combining all geometrical and physical parameters, 1080 cases are run. Just part of the temperature and velocity behaviour is shown here. The concentrations are very small in order to be in agreement with the correlations used for thermal viscosity and thermal conductivity. In a general view, nanofluids proved to smoothly enhance heat transfer as the concentration increases for the range adopted. However, nanoparticle materials play an important role on Nusselt number, being that the highest heat transfer values are for copper.

14/01568 Natural ventilation of buildings due to buoyancy assisted by wind: investigating cross ventilation with computational and laboratory simulation

Stavridou, A. D. and Prinos, P. E. *Building and Environment*, 2013, 66, 104–119.

In this paper cross natural ventilation due to buoyancy assisted by wind is investigated with computational and laboratory simulation. The impact of the outlet's opening position is investigated, forming cross ventilation of variable distance h – namely, the vertical distance between midpoints of leeward and windward opening – for three initial Froude numbers: (i) $Fr_0 = 1.15$, (ii) $Fr_0 = 2.79$ and (iii) $Fr_0 = 4.85$. For the computational simulation a fluid dynamic software is used and the problem is solved by solving the three-dimensional unsteady Reynolds averaged Navier–Stokes equations in conjunction with the energy equation and the turbulence model RNG k-ϵ. The laboratory simulation took place in an open channel and the experimental model represents a building form of orthogonal shape. The interior of the experimental model is filled with solution of ethanol at conditions of normalized gravity, but also with salted water at conditions of inversed gravity. The time taken for the indoor space to empty is calculated numerically and experimentally. Based on Froude number dynamic similarity, the experimental and computational results are characterized by good agreement and the functional process of natural ventilation is being explicated. In addition, the suggestion of using ethanol solution for the density difference between interior and exterior fluid in laboratory simulation of natural ventilation is verified successfully, as the results with use of ethanol solution are in good agreement with those using salted water.

14/01569 Numerical study of conjugate heat transfer of cryogenic methane in rectangular engine cooling channels at supercritical pressures

Wang, L. *et al. Applied Thermal Engineering*, 2013, 54, (1), 237–246.

Three-dimensional conjugate heat transfer of cryogenic methane in rectangular engine cooling channels at supercritical pressures with asymmetric heating imposed on the top channel surface is numerically investigated, focusing mainly on effects of the thermal conductivity of the solid channel material and the geometric aspect ratio of the channel on fluid flow and heat transfer. Results indicate that variations of the thermal conductivity in the solid fin produce significant impact on conjugate heat transfer owing to heat flux redistribution in solid region and convective heat transfer variation in fluid phase. The latter

factor is dictated by strong variations of fluid thermophysical properties at a supercritical pressure. At a constant inlet mass flow rate, variations of the geometric aspect ratio of the channel exert strong influence on both heat transfer and pressure loss due mainly to fluid velocity variations. Results indicate that convective heat transfer plays a more dominating role than thermal conduction in the solid fin. A thermal performance factor can be used for the combined evaluation of heat transfer and pressure loss. The modified Jackson and Hall empirical heat transfer expression is tested to be applicable for heat transfer prediction of cryogenic methane at supercritical pressures.

14/01570 Optimisation for the retrofit of large scale heat exchanger networks with different intensified heat transfer techniques

Pan, M. *et al. Applied Thermal Engineering*, 2013, 53, (2), 373–386.

Intensified heat transfer (IHT) techniques have recently been used for retrofit in the process industry, leading to significant energy saving in heat exchanger network (HEN) by facilitating heat transfer intensification without network topology modification. In this paper, an optimization method has been developed for dealing with the retrofit of large-scale HENs in which the location of intensified heat transfer within the network and its degree of intensification are systematically identified, given the objective function and design constraints, including topological limitation in the existing heat recovery systems. The optimization framework developed is based on iterative optimization of a relatively simple mixed integer linear programming, which can effectively deal with computational difficulties associated with nonlinearity. In the retrofitted HENs, several conventional intensified heat transfer techniques are available, including tube-side intensification (twisted-tape inserts, coiled-wire inserts and internal fins), and shell-side intensification (external fins and helical baffles). Suitable exchangers can be selected for enhancement by implementing one or more intensification techniques to increase the whole network energy recovery within very low retrofit cost. A large-size industrial case study is considered to demonstrate the validity and efficiency of the proposed optimization approach.

14/01571 Passive alternatives to mechanical air conditioning of building: a review

Leo Samuel, D. G. *et al. Building and Environment*, 2013, 66, 54–64.

Human comfort has gained importance in the recent decades. Mechanical air conditioners are the conventional means of creating thermal comfort but they are energy intensive and hence harmful to the environment. Therefore, passive cooling can be adopted as a viable alternative to conventional cooling systems. This paper reviews various passive cooling options available such as nocturnal radiation, geothermal, ventilation, evaporative, hydrogeothermal, deep ocean/lake, thermal insulation and shading along with their advantages, limitations, working principles and climatic dependence. The mathematical equations used for computing the performance of passive cooling systems have been discussed along with design and environmental parameters influencing the systems' performance. The usefulness of phase change materials, thermal mass and radiant cooling in passive cooling systems is also examined. Case studies containing experimental data and numerical predictions are discussed to provide options for building architects and infrastructure developers to adopt the appropriate passive cooling strategy. In addition, issues related to occupants' health and indoor air quality are also explained. A brief review of energy-efficient and eco-friendly solar cooling systems is also included.

14/01572 PCMs inside emulsions: some specific aspects related to DSC (differential scanning calorimeter)-like configurations

Kousksou, T. *et al. Energy*, 2013, 56, 175–183.

The heat transfer characteristics during melting of the phase change material (PCM) dispersed inside an emulsion are investigated theoretically and experimentally by using differential scanning calorimeter. Genetic algorithm is used to determine the unknown parameters in the physical model. The dispersed PCMs are hexadecane, heptadecane and octadecane. Energy analysis is carried out to understand the thermal behaviour of the simple and mixed emulsions. The effect of the heating rate on the thermal behaviour of emulsion is also analysed.

14/01573 Performance comparison of the plate heat exchanger using different nanofluids

Tiwari, A. K. *et al. Experimental Thermal and Fluid Science*, 2013, 49, 141–151.

An effort has been made to compare experimentally the heat transfer performances of various nanofluids. The heat transfer performance of the plate heat exchanger have been investigated using different nanofluids (CeO_2, Al_2O_3, TiO_2 and SiO_2) for various volume flow rates and wide range of concentrations. Optimum concentrations for different nanofluids have been determined as well, which yields maximum heat transfer improvement over base fluid. Prior to the experiments, the required thermophysical properties of the nanofluids were measured. The performance has been discussed in terms of overall heat transfer coefficient ratio, heat transfer coefficient ratio, pressure drop ratio, pumping power ratio, effectiveness ratio and performance index ratio. Study showed that CeO_2/water yields best performance (maximum performance index enhancement of 16%) with comparatively lower optimum concentration (0.75 vol.%) within studied nanofluids.

14/01574 Performance evaluation of a two-stage compression heat pump system for district heating using waste energy

Kwon, O. *et al. Energy*, 2013, 57, 375–381.

The present study investigated a two-stage compression heat pump system for district heating utilizing waste energy. An evaporator and condenser exhibit a large difference in temperature when hot water is produced for heating by a heat pump. With single-stage compression, this causes a dramatic drop in the compressor efficiency and lowers the system performance; so, in the present study, a two-stage compression heat pump system comprising an intercooler and flash tank was designed, and the performance characteristics under various operating conditions were tested. When the heat source temperature was raised from 10 to 30 °C, the coefficient of performance was improved by up to 22.6%. As the superheating at the low-stage compressor was increased from 2 to 11 °C, the refrigerant flow rate and heating capacity decreased by as much as 7.6% and 2.2%, respectively, but there was no major impact on the temperature of the hot water produced nor on the system performance. Controlling the frequency of the high-stage compressor to control the intermediate pressure resulted in the ability to improve performance by as much as 5.2% under identical heat source conditions.

14/01575 Root zone temperature control with thermal energy storage in phase change materials for soilless greenhouse applications

Beyhan, B. *et al. Energy Conversion and Management*, 2013, 74, 446–453.

A new root zone temperature control system based on thermal energy storage in phase change materials (PCM) has been developed for soilless agriculture greenhouses. The aim was to obtain optimum growing temperatures around the roots of plants. The candidate PCMs were 40% oleic acid–60% decanoic acid mixture and oleic acid alone. Field experiments with these PCMs were carried out in November 2009 with *Cucurbite pepo* and in March 2010 with *Capsicum annum* plants. No additional heating system was used in the greenhouse during these periods. In the November 2009 tests with zucchini, 40% oleic acid + 60% capric acid mixture was the PCM and a temperature increase in the PCM container (versus the control container) was measured as 1.9 °C. In the March 2010 tests with peppers, both PCMs were tried and the PCM mixture was found to be more effective than using oleic acid alone. A maximum temperature difference achieved by the PCM mixture around the roots of peppers was 2.4 °C higher than that near the control plants.

14/01576 Self-heating Schottky emission from a ballasted carbon nanotube array

Sun, Y. *et al. Carbon*, 2013, 58, 87–91.

A ballast resistor is utilized in a low density vertically aligned carbon nanotube (CNT) array. Based on the nature of the ballast resistor, the uniformity of the emission improves remarkably. A highly stable field emission current is obtained under a constant voltage and a current density of 300 mA/cm^2 is achieved. Joule heat generated by this field emission current increases the temperature of the CNT array significantly. The high temperature changes the emission to Schottky emission regime. The Schottky emission achieves 900 mA/cm^2, which is three times the field emission current density. A simulation result shows the corresponding temperature is about 1700 K. A colour change of the emission area is observed after the experiment. When compared to the conventional Schottky cathode, the emitter is self-heating and no extra heater is needed. This is the first report of a successful utilization of a ballast resistor in a CNT based emission array and the first observation of Schottky emission from a vertically aligned CNT array used as an electron emitter.

14/01577 Study of the heat transfer and flow resistance of large and small hole (LASH) baffle heat exchanger

Sun, H. and Qian, C. *Applied Thermal Engineering*, 2013, 54, (2), 536–540.

In this study, heat transfer and flow resistance properties of large and small hole (LASH) baffle heat exchangers are studied with experimentally verified numerical models. Effects of the large-hole diameters and baffle pitches are investigated. Results show that as a result of parallel flow, the shell-side pressure drops of the LASH baffle heat exchangers are greatly decreased compared with that of the conventional segmental baffle heat exchanger for the same baffle pitch.

If the large-hole diameter and baffle pitch are properly chosen, the LASH baffle heat exchanger presents a larger shell-side heat transfer coefficient and lower shell-side pressure drop. For the same shell-side pressure drop, the shell-side heat transfer coefficients of the LASH heat exchangers can be increased by as much as 25% compared with the conventional segmental baffle heat exchanger.

14/01578 Temperature response functions (*G*-functions) for single pile heat exchangers

Loveridge, F. and Powrie, W. *Energy*, 2013, 57, 554–564.

Foundation piles used as heat exchangers as part of a ground energy system have the potential to reduce energy use and carbon dioxide emissions from new buildings. However, current design approaches for pile heat exchangers are based on methods developed for boreholes which have a different geometry, with a much larger aspect (length to diameter) ratio. Current methods also neglect the transient behaviour of the pile concrete, instead assuming a steady state resistance for design purposes. As piles have a much larger volume of concrete than boreholes, this neglects the significant potential for heat storage within the pile. To overcome these shortcomings this paper presents new pile temperature response functions (*G*-functions) which are designed to reflect typical geometries of pile heat exchangers and include the transient response of the pile concrete. Owing to the larger number of pile sizes and pipe configurations which are possible with pile heat exchangers it is not feasible to developed a single unified G-function and instead upper and lower bound solutions are provided for different aspects ratios.

14/01579 The comparison of designed water-cooled and air-cooled passive residual heat removal system for 300 MW nuclear power plant during the feed-water line break scenario

Wang, M. *et al. Annals of Nuclear Energy*, 2013, 57, 164–172.

The steam generator (SG) secondary water-cooled and air-cooled passive residual heat removal systems (PRHRSs) are proposed and designed for 300 MW pressurized water reactor (PWR). The RELAP5/MOD3.4 code is utilized to study the behaviour of the PRHRSs and transient characteristics of primary loop system during feed-water line break accident. The characteristic comparison between water-cooled and air-cooled PRHRSs is also conducted in this study. The results show that both water-cooled and air-cooled PRHRSs can establish stable natural circulations in PRHRS loops, which realize the effective core decay heat removal from primary loop. Results illustrate that both water-cooled PRHRS and air-cooled PRHRS designed in the study have great significance for improving the inherent safety of 300 MW nuclear power plant. However, the water-cooled PRHRS heat transfer ability is stronger in the initial time, while it becomes weaker as the system tank water evaporates in the later stage. In contrast, the air-cooled PRHRS, ensuring the main reactor operation parameters to decrease to a more safety value, is more effective than water-cooled PRHRS for long-term cooling.

14/01580 The design and simulation of a new spent fuel pool passive cooling system

Ye, C. *et al. Annals of Nuclear Energy*, 2013, 58, 124–131.

Due to the safety issues arising from the Fukushima accident, a novel completely passive spent fuel pool cooling system is proposed using the high-efficiency heat pipe cooling technology that is available in an emergency condition such as a station blackout. This cooling system's ability to remove the decay heat released by the spent fuel assemblies is evaluated by a computational fluid dynamics simulation. The spent fuel pool of CAP1400 (a passive pressurized water reactor developed in China) is selected as the reference pool, and the passive cooling system is designed for this spent fuel pool. The pool with the passive cooling system is simulated using Fluent 13.0 with four million meshes. Four different cases have been studied, and some notable results have been obtained through this work. The simulation results reveal that the passive cooling system effectively removes the decay heat from the spent fuel pool with the storage of 15-year-old spent fuel assemblies and prevents the burnout of the fuel rods. The results indicate that the water in the spent fuel pool will never boil, even in a severe accident with a lack of emergency power and outside aid.

14/01581 The Diavik Waste Rock Project: measurement of the thermal regime of a waste-rock test pile in a permafrost environment

Pham, N. H. *et al. Applied Geochemistry*, 2013, 36, 234–245.

The interior thermal regime of a field-scale experimental waste rock pile in the Northwest Territories, Canada, was studied. Test pile construction was completed in the summer 2006, and temperature data were collected continuously since that time to February 2009. The temperature data indicate the test pile cooled over the study period, with an average heat energy release of -2.5×10^4 and -2.6×10^4 MJ in 2007 and 2008, respectively. The mean annual air temperature (MAAT) at the site was −8.9 °C during the period between 2006 and 2009, with a permafrost table at a depth of 4 m in bedrock away from the pile. Because of this cold environment, the upward movement rate of the 0 °C isotherm into the test pile at its base was approximately 1.5 m a^{-1} during 2007 and 2008. Thermistor strings installed immediately below the base of the test pile showed the test-pile basal temperatures remained near and below 0 °C during the study period. Furthermore, due to low rates of sulfide mineral oxidation, elevated temperatures in the interior of the test pile were not observed. The average air velocity in the pore space in July 2007 and 2008 was about one-third of that during January of each year based on temperature distributions. Therefore, due to higher air velocity during the winter, it is expected that heat transfer is greater during winter.

14/01582 The present and future of residential refrigeration, power generation and energy storage

Wang, R. Z. *et al. Applied Thermal Engineering*, 2013, 53, (2), 256–270.

Based on the fast development of energy efficiency, energy safety and use of renewable and sustainable energy, various energy systems related to residential refrigeration, power generation and storage have been developing. Some of them are in large-scale application, while others are still under development. Current status of residential refrigeration, power generation and energy storage technologies have been briefly summarized in this paper. Also, future residential refrigeration, power generation and energy storage technologies are highlighted, and some roadmaps are discussed.

14/01583 The role of pumped and waste heat technologies in a high-efficiency sustainable energy future for the UK

Markides, C. N. *Applied Thermal Engineering*, 2013, 53, (2), 197–209.

This paper begins with an overview of the current supply and demand characteristics of primary energy for the provision of heat and power in the UK. This is followed by a brief review of a variety of solutions that are being proposed towards the establishment of a sustainable energy landscape, including clean coal, wind and solar energy. The discussion extends to the economics and performance of various renewable energy systems in comparison to fossil fuel equivalents. Placed in this context, the study then focuses specifically on the role of pumped heat, combined heat and power (CHP) schemes, and options for the recovery and conversion of waste heat into useful work, all of which have a potential to contribute towards the creation of a 'high-efficiency sustainable energy future'. It is concluded that although the problem is complex, the relative costs of competing technologies are not prohibitive, but comparable, leading to an inability to make a decisive choice and delaying progress. CHP and pumped heat are found to be similar in terms of overall efficiency, with the load factor (heat-to-power demand ratio) being of critical importance. Various waste heat conversion systems are also found to be similar in terms of the important indicator of power per unit cost.

14/01584 Thermal optimization of PCM based pin fin heat sinks: an experimental study

Baby, R. and Balaji, C. *Applied Thermal Engineering*, 2013, 54, (1), 65–77.

This paper reports the results of an experimental investigation carried out to characterize the thermal performance of different configurations of phase change material (PCM)-based pin-fin heat sinks. Paraffin wax and n-eicosane are used as the PCMs. Aluminium is used to make the heat sinks and the volume fraction is varied by changing the number of pin fins. Baseline comparisons are done with a heat sink filled with PCM, without any fin. The effect of PCM volume fraction on the heat transfer performance is also studied. The results showed that there exists sufficient scope to optimize the thermal design of the heat sink. An artificial neural network–genetic algorithm hybrid algorithm is then developed to determine the optimum configuration of the pin-fin heat sink that maximizes the operating time for the n-eicosane-based heat sink. The resulting optima was found to be valid even for the paraffin wax-based PCM.

14/01585 Thermal performance of elliptical pin fin heat sink under combined natural and forced convection

Deshmukh, P. A. and Warkhedkar, R. M. *Experimental Thermal and Fluid Science*, 2013, 50, 61–68.

In this paper, the effects of design parameters have been experimentally investigated for the air side thermal performance under mixed (combined natural and forced) convection of the fully shrouded elliptical pin fin heat sinks and the values of optimum design parameters are sought. A theoretical model is used to predict the influence of various geometrical, thermal and flow parameters on the thermal resistance of the heat sink. An experimental measurement technique is utilized to indirectly measure the overall heat transfer coefficient of the heat sink in mixed convection with assisting flow. The thermal performance characteristics are obtained for various parameters with inline and staggered layout of the pin fin heat sinks resulting in optimum heat sink void fraction (α), and pin fin aspect ratio (Υ). The comparative thermal performances of circular and

elliptical profiled pin fin heat sinks are presented. Based on experimental data for the range of fin, air flow and heat sink parameters, with aspect ratio, $5.1 \leq \Upsilon \leq 9.18$; heat sink void fraction, $0.534 \leq \alpha \leq 0.884$; approach velocity, $0.1 \leq U_{infin} \leq 0.5$; longitudinal fin pitch, $18 \leq S_L \leq 36$ mm; transverse fin pitch, $9 \leq S_T \leq 18$ mm; elliptical pin fin axis ratio $\varepsilon = 0.66$ and mixed convection parameter, $1 \leq Gr_d/Re_d \leq 100$; generalized empirical correlations are developed for elliptical pin fin heat sink.

11 ENGINES

Power generation and propulsion, electrical vehicles

14/01586 Analysis of recoverable exhaust energy from a light-duty gasoline engine

Wang, T. *et al. Applied Thermal Engineering*, 2013, 53, (2), 414–419.

While exhaust energy recovery (EER) has been widely studied for improving the total efficiency and reducing CO_2 emissions of internal combustion engines, the improvement on engine efficiency has been investigated with experimental work and numerical simulation based on a steam Rankine cycle EER system. The test was conducted on a light-duty gasoline engine connected with a multi-coil helical heat exchanger. Combining those experimental and modelling results, it demonstrates that the flow rate of working fluid plays a very important and complex role for controlling the steam outlet pressure and overheat degree. For achieving required overheat and steam pressure, the flow rate must be carefully regulated if the engine working condition changes. The flow rate has also significant influence on the heat exchanger efficiency. To achieve better heat transfer efficiency, the flow rate should be maintained as high as possible. From the simulation, it is found the EER system based on the light-duty test engine could increase the engine fuel conversion efficiency up to 14%, though under general vehicle operating conditions it was just between 3% and 8%. From the test, it is found the installation of heat exchanger can increase the exhaust back pressure slightly, the total fuel saving of the engine could be up to 34% under some operating condition.

14/01587 Conversion of a heavy duty truck diesel engine with an innovative power turbine connected to the crankshaft through a continuously variable transmission to operate compression ignition dual fuel diesel-LPG

Boretti, A. *et al. Fuel Processing Technology*, 2013, 113, 97–108.

This paper considers the option to convert the diesel engine to liquid petroleum gas (LPG) retaining the diesel-like behaviour. LPG is an alternative fuel with a better carbon to hydrogen ratio permitting reduced carbon dioxide emissions. It flashes immediately to gaseous form even if injected in liquid state for a much cleaner combustion almost cancelling some of the emissions of the diesel. Within Australia, LPG permits a much better energy security and the refuelling network is widespread. In this paper, a latest heavy duty truck diesel engine with a novel power turbine connected through a continuously variable transmission to the crank shaft and fitted with a by-pass is modified to accommodate a second direct injector for the LPG fuel and operate full load with 5% diesel and 95% LPG. Results of engine performance simulations with diesel and diesel–LPG are presented. The engine retains the diesel performances while permitting the advantages of LPG in terms of particulate, carbon dioxide emissions and diversification of fuel supplies and energy security.

14/01588 Effect of partial-heating of the intake port on the mixture preparation and combustion of the first cranking cycle during the cold-start stage of port fuel injection engine

Li, T. *et al. Experimental Thermal and Fluid Science*, 2013, 49, 14–21.

For port fuel injection (PFI) engines, excessive fuel is needed for the first few cycles during the cold-start because of the unfavourable evaporation environment. The excessive fuel usually forms a fuel film which causes non-uniform mixture and becomes a major source of the engine-out hydrocarbons (EOHC). In this paper, a partial-heating method was proposed to improve the evaporation of the deposited fuel film at the beginning of the cold-start of PFI engine. The partial-heating method focuses on increasing the surface temperature of the intake port end before the cranking start. In this study, the effect of the partial-heating was researched based on the first cranking cycle. The effect was experimentally investigated and discussed in terms of the mixture preparation, combustion and EOHC. The results showed that within the capacity of the on-board battery, the partial-heating led to efficient and effective heating of the surface of the intake port end. The fuel delivery efficiency was increased by over 10%. Fuel enrichment was reduced from 40 to 30 ms FPW within 15 s of the partial-heating. Moreover, the mixture was found to burn faster in the partial-heating cases. Higher indicated mean effective pressure could be obtained with optimized spark timing in the partial-heating cases.

14/01589 Experimental investigation into the effects of two-stage injection on fuel injection quantity, combustion and emissions in a high-speed optical common rail diesel engine

Herfatmanesh, M. R. *et al. Fuel*, 2013, 109, 137–147.

Diesel combustion and the formation of pollutants are directly influenced by the spatial and temporal distributions of the fuel within the combustion chamber of an internal combustion engine. The requirements for more efficient and responsive diesel engines have led to the introduction and implementation of multiple injection strategies. However, the effects of such injection modes on the hydraulic systems, such as the high pressure pipes and fuel injectors, must be thoroughly examined and compensated for. The objective of this study was to investigate the effects of fuel injection equipment characterization and optimization on diesel combustion and emissions with two-stage fuel injection. The fuel injection system was characterized and optimized through the measurement of the fuel injection rate and quantity, in particular, the interaction between the two injection events was quantified and compensated for. The effects of twin and variable split two-stage injection and dwell angle on diesel combustion and emissions were investigated in a high-speed direct injection single-cylinder optical diesel engine using heat release analysis and high-speed fuel spray and combustion visualization technique. The results indicated that two-stage injection has the potential for simultaneous reduction of NO_x and soot emissions. Nevertheless, the studied two-stage strategies resulted in higher soot emission, mainly due to the interaction between two consecutive fuel injection events, whereby the fuel sprays during the second injection were injected into burning regions, generating fuel-rich combustion. In addition, the variable two-stage strategies produced high levels of uHC emission in comparison to single and twin split injection cases. This was mainly attributed to firstly greater fuel quantity injected during the second injection and secondly poor mixing and air utilization during the second fuel injection event.

14/01590 Experimental study on energy and exergy analyses of a diesel engine performed with multiple injection strategies: effect of pre-injection timing

Özkan, M. *et al. Applied Thermal Engineering*, 2013, 53, (1), 21–30.

Several studies in the literature treat the effects of ambient conditions and alternative fuel usage on the thermal and exergetic efficiencies of diesel engines. Differently to other studies, this study investigates the influence of the dwell time of multiple injection events on the thermal and exergetic efficiencies. A test engine was run using three different injection strategies. The main injection timing, the total fuel injected into the combustion chamber per cycle, the engine speed, the rail pressure and the intake manifold pressure were held constant, and the pre-injection timing was varied during the engine tests. Using the results of the engine experiments, the heat release rate, combustion temperature, heat balance, thermal efficiency, and exergetic efficiency were calculated. While no significant change in the thermal efficiency was obtained, exergetic efficiency and the exergy, the NO_x emissions decreased by 7.4% via implementing appropriate pre-injection mass and injection advance. The combustion temperature and cooling heat loss decreased, while the exhaust heat loss increased when using the pre-injection strategies. The results demonstrate that pre-injection strategies, whose main goal is reducing NO_x emissions, cause negligible losses in the thermal and exergetic efficiencies.

14/01591 Frequency based approach for simulating pressure waves at the inlet of internal combustion engines using a parameterized model

Mezher, H. J. *et al. Applied Energy*, 2013, 106, 275–286.

Today's downsized turbocharged engines mainly focus on improving low end torque and increasing mass flow rate, this is done in order to improve the overall thermodynamic efficiency of the engine and to gain a lower brake specific fuel consumption. An integral part of any combustion engine is the air intake line that has a first-order effect on engine filling and emptying. The wave action that takes place is usually simulated using one-dimensional codes. This paper presents a novel technique based on a frequency domain characterization of the intake line. A link over a wide frequency spectrum is identified between the instantaneous mass flow at the valve and the dynamic pressure response. This model is implemented into Simulink via a transfer function and coupled to GT-Power to produce an engine simulation. A shock tube experimental campaign was conducted for a number of tubes with varying lengths and diameters. The parameters of this

transfer function are measured for each case then combined with gas dynamic theory and a frequency analysis to identify a law of behaviour as a function of pipe geometry. The final model is validated on a single cylinder engine in GT-Power for a variety of pipe geometry.

14/01592 Impact of idling on fuel consumption and exhaust emissions and available idle-reduction technologies for diesel vehicles – a review

Rahman, S. M. A. *et al. Energy Conversion and Management*, 2013, 74, 171–182.

In order to maintain cab comfort, truck drivers have to idle their engines to obtain the required power for accessories such as air-conditioning, heating, television, refrigerator and lighting. This idling of the engine has a major impact on its fuel consumption and exhaust emissions. Idling emissions can be as high as 86.4, 16,500, 5130, 4 and 375 g/h for HC, CO_2, CO, particulate matter and NO_x, respectively. Idling fuel consumption rate can be as high as 1.85 gal/h. The accessory loading, truck model, fuel-injection system, ambient temperature, idling speed, etc., also affect significantly the emission levels and fuel consumption rate. An increase in accessory loading and ambient temperature increases the emissions and fuel consumption. During idling, electronic fuel-injection systems reduce HC, particulate matter and CO emission, but increase NO_x emissions compared with a mechanical fuel-injection system. An increase of idling speed increases fuel consumption rate. There are many systems available on the market to reduce engine idling and improve air quality and fuel consumption rate, such as an auxiliary power unit (APU), truck stop electrification, thermal storage systems, fuel cells, and direct fire heaters. A direct fire heater reduces fuel consumption by 94–96% and an APU reduces consumption by 60–87%. Furthermore, these technologies increase air quality significantly by reducing idling emissions, which is the reason why they are considered as key alternatives to engine idling.

14/01593 Simultaneous imaging of diesel spray atomisation and evaporation processes in a single-cylinder CR diesel engine

Herfatmanesh, M. R. *et al. Experimental Thermal and Fluid Science*, 2013, 50, 10–20.

In direct injection diesel engines, combustion and formation of pollutants are directly influenced by the spatial and temporal distributions of the injected fuel. In this study mixture formation during the pre-combustion phase of a diesel engine was investigated using the laser-induced exciplex fluorescence (LIEF) technique. The main purpose of this investigation was to develop an experimental setup capable of providing the full-field view of both liquid and vapour phases of evaporating diesel sprays during the fuel injection process inside the combustion chamber of a diesel engine with optical access. An expanded laser beam was employed for full combustion chamber visualization. In this study two model fuels were tested; one consisted of 89% decane, 10% α-methyl-naphthalene and 1% TMPD and the other 88% decane, 10% α-methyl-naphthalene and 2% TMPD. The spray atomization and evaporation processes during the pre-combustion phase of a diesel engine were measured at an injection pressure of 1200 bar and the engine speed of 1500 rpm. The results demonstrated the capability of the full-field LIEF technique in simultaneous imaging of liquid fraction and fuel vapour distribution during high pressure fuel injection process. It also highlighted the effect of dopant concentration on the fluorescence intensity of liquid and vapour signals. The exciplex system containing 1% TMPD produced better visualization of the liquid phase, though the crosstalk in the vapour phase precluded accurate detection of the vapour phase signal. In contrast, the exciplex system containing 2% TMPD resulted in satisfactory visualization of the vapour phase; however the intensity of the liquid phase was compromised as a result. This was presumed to be mainly due to the spectral shift of the exciplex species and/or TMPD decomposition at elevated temperatures and pressures.

14/01594 The role of heat exchange on the behaviour of an oscillatory two-phase low-grade heat engine

Solanki, R. *et al. Applied Thermal Engineering*, 2013, 53, (2), 177–187.

A particular type of oscillatory low-grade heat engine is examined with specific attention to the two-phase heat transfer process undergone in the device during operation. Three linear and spatially lumped models of this device are investigated, which incorporate: (a) a linear temperature profile (LTP) in the heat exchangers; (b) a constant temperature difference (CTD) between the heat exchangers and working fluid; and (c) a dynamic ability of the heat exchanger (DHX) blocks to store and release heat periodically. The LTP model has been presented in earlier work, where it was shown that including the effects of liquid flow inertia was important in the modelling of the device. In this paper, the CTD and DHX models are developed and probed in order to study the effects of alternative heat exchange assumptions and descriptions on the operation and performance of the device. The condition for which continuous, sustained oscillations occur in the three models (i.e. marginal stability) and their associated exergetic efficiencies at this condition are calculated and compared. It is found that all three models predict oscillation frequencies in the same order of magnitude, but that the CTD model predicts unrealistically high efficiencies. Interestingly, when parameters associated with the power cylinder of the device are varied, a discontinuity in the oscillation frequency of the system is observed with all models. This feature has not been reported previously and is important for the better understanding and, ultimately, the improved design of such devices.

Hybrid engine systems

14/01595 An experimental investigation of effect on diesel engine performance and exhaust emissions of addition at dual fuel mode of hydrogen

Köse, H. and Ciniviz, M. *Fuel Processing Technology*, 2013, 114, 26–34.

Internal combustion engines are an indispensable part of our daily life, especially in transportation and agriculture sectors. However, the reduction of petroleum resources and environmental problems are leading to an increasing trend towards alternative energy sources. In this regard, hydrogen usage is expected to be a solution for previously mentioned problems as one of the renewable energy resources. In this concept, effects of hydrogen as an additional fuel used in a compression ignition engine performance and exhaust emissions parameters different engine speeds were investigated at full load. For this purpose, a compression ignition engine with 17/1 compression ratio, four cylinders, four stroke, turbocharger and 3.908-litre engine volume was used. While diesel fuel was injected directly to combustion chamber, hydrogen was added to inlet manifold at rates of 2.5%, 5% and 7.5% as volume. As a result, an increase in engine torque, power, thermal efficiency, nitrogen oxides (NO_x) and exhaust gasses temperatures were acquired at every hydrogen addition ratio while a decrease in hydrocarbon, carbon monoxide and oxygen emissions were attained. While engine torque exhibited an increase at a rate of 8.3% comparing with standard diesel operation at 1250 min^{-1} and 7.5% hydrogen addition ratio, engine power increased 17% at 2250 min^{-1} engine speed and 7.5% hydrogen addition ratio. Brake thermal efficiency of 2.5% was obtained as 40.4% comparing with 33% value of SDI at 1750 min^{-1}. The lowest CO, CO_2, HC and NO_x emission values were obtained at 2250 min^{-1} engine speed and 2.5% hydrogen addition ratio as 0.013; 2500 min^{-1} engine speed and 7.5% hydrogen addition ratio as 7.4%; 1250 min^{-1} engine speed and 2.5% hydrogen addition ratio as 10 ppm and 1000 min^{-1} engine speed and 7.5% hydrogen addition ratio as 1092 ppm respectively comparing with standard diesel operation.

14/01596 Combustion and emissions characteristics of a dual fuel engine operated on alternative gaseous fuels

Mustafi, N. N. *et al. Fuel*, 2013, 109, 669–678.

Among the different efforts towards the reduction in pollutant emissions from direct injection (DI) diesel engines, the use of gaseous fuels as a partial supplement for diesel fuel has been proposed by many researchers. An experimental investigation was performed to investigate the influence of dual-fuel combustion on the performance and exhaust emissions of a DI diesel engine fuelled with natural gas (NG) and biogas (BG). The engine was operated at a constant speed of 1750 rpm and at two different loads: low (~3 N m) and high (~28 N m), which were about 10% and 85%, respectively, of the rated torque output of the engine at 1800 rpm. In this work, the combustion pressure and the rate of heat release were evaluated experimentally in order to analyse the combustion characteristics and their effects on exhaust emissions including particulate matter (PM) for single-fuel (diesel) and dual fuel combustion modes. In dual fuel mode, the peak cylinder pressure was found to be similar to diesel at 75% of the rated output of the engine. About 27–30% higher maximum net heat release rates were obtained for NG and biogas fuelling, respectively, compared to diesel fuelling. Longer ignition delays but shorter combustion durations were characterized for dual fuelling operations. Specific NO_x emissions for dual fuelling was always lower than diesel fuelling case. Significantly lower specific PM emissions but sharply increased unburned hydrocarbons emissions were measured for biogas–diesel dual fuel operations as compared to diesel fuelling.

14/01597 Dimethyl ether energy ratio effects in a dimethyl ether-diesel dual fuel premixed charge compression ignition engine

Wang, Y. *et al. Applied Thermal Engineering*, 2013, 54, (2), 481–487.

The combination of port dimethyl ether (DME) induction and in-cylinder diesel direct-injection compression ignition combustion was studied in a two-cylinder engine. The port DME energy ratio was proved to be one of main variables affecting the combustion. Thus, the

main goals of this paper were to investigate the effects of DME energy ratio on combustion and emission characteristics of the diesel engine at this dual-fuel PCCI combustion mode. In order to evaluate the characteristics of this combustion mode, the conventional direct-injection compression ignition engine performance was provided to make a detailed comparison. Furthermore, special concern was focused on the complex combustion process analysis. DME port induction and diesel in-cylinder direct-injection combustion process was composed of the homogeneous charge compression ignition combustion and conventional diffusive combustion. Although DME energy ratio had little impact on the start timing of cool flame, the negative temperature coefficient region shortened and the start timing of HCCI high-temperature reaction advanced as DME energy ratio increased. It could also be discovered that, as DME energy ratio increased, the maximum heat release rate of DME HCCI increased as well as the peak values of cylinder pressure and mass-averaged temperature; however, the maximum heat release rate of diesel combustion decreased. Results also showed the brake thermal efficiency slightly increased with a rise of DME energy ratio. In the case of emission, smoke emissions decreased, NO_x emissions decreased first but this decreasing trend was inhibited later, while HC and CO emissions increased with a rise of DME energy ratio.

14/01598 Hydro-pneumatic accumulators for vehicles kinetic energy storage: influence of gas compressibility and thermal losses on storage capability

Puddu, P. and Paderi, M. *Energy*, 2013, 57, 326–335.

In this work the differences between the thermodynamic behaviour of real and ideal gases are analysed to determine their influence on the processes of compression and expansion of a gas-charged accumulator. The behaviour of real gas has a significant influence on the size of accumulators used for kinetic energy recovery of vehicles. In particular, it is underscored that the accumulator's design, based on ideal gas behaviour, provides undersized accumulators and therefore makes impossible the complete energy recovery for hydraulic energy storage systems. The analysis of the thermodynamic properties of gases has shown that the main differences between ideal and real behaviour are due to gas compressibility. A mathematical model of a gas-charged accumulator is developed in order to analyse its real behaviour in presence of irreversible heat transfer and viscous losses. The simulation process of charging and discharging of a hydro-pneumatic accumulator, makes it clear that hydrodynamic and thermal losses are responsible for the characteristic hysteresis cycle on the p–V diagram. Different gases are tested as charged fluid of a hydro-pneumatic accumulator to simulate cyclic processes of charge and discharge. Results show different characteristics in terms of volumetric gas properties, thermal time-constant and thermal efficiency of the accumulator.

Transport battery development

14/01599 Energy efficiency and capacity retention of Ni–MH batteries for storage applications

Zhu, W. H. *et al. Applied Energy*, 2013, 106, 307–313.

The Ni–MH batteries were tested for battery energy storage characteristics, including the effects of battery charge or discharge at different rates. The battery energy efficiency and capacity retention were evaluated through measuring the charge/discharge capacities and energies during full and partial state-of-charge (SoC) operations. Energy efficiency results were obtained at various charge input levels and different charge and discharge rates. The inefficient charging process started to take place at *ca.* 90% state-of-recharge (SoR) when charged at no more than 0.2 C rate. For the NiMH-B2 battery after an approximately full charge (~100% SoC at 120% SoR and a 0.2 C charge/discharge rate), the capacity retention was obtained as 83% after 360 h of storage, and 70% after 1519 h of storage. The energy efficiency was decreased from 74.0% to 50% after 1519 h of storage time. The Coulomb efficiency was initially 83.34%, and was reduced to 57.95% after 1519 h of storage. The battery has relatively higher energy efficiency at approximately 50% SoC. The energy efficiency was calculated to be more than 92% when the NiMH-C3 battery was charged to 30–70% SoC then discharged to 0% SoC at a 0.2 C charge/discharge rate. In consideration of energy efficiency, charge acceptance, capacity retention rate, and power output needs, as well as Nelson's analysis on HEV power requirements, the Ni–MH battery is appropriate to work at *ca.* 50 ± 10% SoC with an operating limitation of 50 ± 20% SoC. This work is potentially beneficial for determination of the current SoC level during the battery pack being operated for energy storage applications.

14/01600 In-plane ordering of Li species in the interlayer of the turbostratic carbon as negative electrode for a high-power and long-life Li ion battery

Fujimoto, H. and Morita, K. *Carbon*, 2013, 56, 317–323.

The fundamental electrochemical performances of a new carbon called ICOKE which was prepared by the graphitization of coke at *ca.* 2000 °C were recently reported. It showed the excellent pulse charge/discharge characteristics and long cycle performance. In the present study, the in-plane structure of Li-intercalated ICOKE was investigated in detail by means of cyclic voltammetry, X-ray diffraction profile change and the Li-NMR spectra. As a result, it was found that the ionic state of Li species in the interlayer and the in-plane structure of Li-intercalated ICOKE were different from those of natural graphite.

14/01601 One-pot synthesis of uniform Fe_3O_4 nanocrystals encapsulated in interconnected carbon nanospheres for superior lithium storage capability

Zhao, N. *et al. Carbon*, 2013, 57, 130–138.

Uniform and small Fe_3O_4 nanocrystals (~9 nm) encapsulated in interconnected carbon nanospheres (~60 nm) for a high-rate Li-ion battery anode have been fabricated by a one-step hydrothermal process followed by annealing under Ar, which can be applied for the preparation of a number of metal oxide nanocrystals encapsulated in interconnected carbon nanospheres. The as-synthesized interconnected Fe_3O_4@C nanospheres displayed high performance as an anode material for Li-ion battery, such as high reversible lithium storage capacity (784 mA h/g at 1 C after 50 cycles), high Coulombic efficiency (~99%), excellent cycling stability, and superior rate capability (568 mA h/g at 5 C and 379 mA h/g at 10 C) by virtue of their unique structure: the nanosized Fe_3O_4 nanocrystals encapsulated in interconnected conductive carbon nanospheres not only endow large quantity of accessible active sites for lithium ion insertion as well as good conductivity and short diffusion length for lithium ion transport but also can effectively circumvent the volume expansion/contraction associated with lithium insertion/extraction.

14/01602 Reduced graphene oxide with tunable C/O ratio and its activity towards vanadium redox pairs for an all vanadium redox flow battery

Li, W. *et al. Carbon*, 2013, 55, 313–320.

Electrochemically reduced graphene oxides (ERGO) are obtained under various reducing potentials in the phosphate buffer solution (PBS). Different characterization methods are used to analyse the changes of structure and surface chemical condition for graphene oxide (GO). The results show that GO could be reduced controllably to certain degree and its electrochemical activity towards VO_2^+/VO^{2+} and V^{3+}/V^{2+} redox couples is also tuneable using this environmentally friendly method. The catalytic mechanism of the ERGO is discussed in detail, the C=O functional groups other than the C–O functional groups on the surface of ERGO more likely provide reactive sites for those redox couples, leading to a more comprehensive understanding about the catalytic process than previous relevant researches. This controllable modification method and the ERGO as electrode reaction catalyst with enhanced battery performance are supposed to have promising applications in the all vanadium redox flow battery.

14/01603 Screening process-based modeling of the multi-cell battery string in series and parallel connections for high accuracy state-of-charge estimation

Kim, J. and Cho, B. H. *Energy*, 2013, 57, 581–599.

This paper investigates a practical universal modelling of multi-cell battery strings in series and parallel connections to show high an accuracy state-of-charge (SOC) estimation based on the extended Kalman filter (EKF) if cell-to-cell variations are taken into account and settled by the screening process. Through the screening process for the selection of the cells that have similar electrochemical characteristics, this study describes an effort to provide each equivalent circuit model for multi-cell battery strings in series, parallel, and series/parallel connections. Three circuit-based multi-cell battery models are validated against the experimental data of the discharging/charging behaviour in terms of the discharging/charging voltage, discharge capacity, open-circuit voltage (OCV), and internal resistances when compared with the experimental data of a single cell. According to the relation between a multi-cell battery string and a single cell, these models can be easily developed from a single cell model, the validity of which was demonstrated regarding its high accuracy in predicting cell performance. The proposed multi-cell battery model has been extensively validated by the model-based SOC estimation using the EKF for a Li-ion cell. If the model parameters of a single cell are correctly measured and used in the multi-cell battery model, the accuracy in the SOC estimation of a multi-cell battery string could be significantly improved.

12 REFRACTORIES/ CERAMICS

Properties, production, applications

14/01604 Effect of γ-irradiation on optical absorption of Al_2O_3–TeO_2–$Li_2B_4O_7$ glasses doped with MgF_2

Farouk, M. *et al. Annals of Nuclear Energy*, 2013, 56, 39–43.

The effect of γ-radiation on the optical properties of the glassy system [$x$$MgF_2$–10$Al_2O_3$-(40-$x$) TeO_2–50$Li_2B_4O_7$], (x = 0, 15, 20 and 40 mol%) has been investigated. Samples were prepared by conventional melt-quench technique. The density and molar volume were estimated and found to decrease with increasing MgF_2 concentration. The obtained data indicate that the glass structure becomes less tightly packed with increasing the MgF_2 concentration. The effect of γ-irradiation (5, 20, 40 and 70 kGy) on optical absorption has been studied. It was observed that γ-radiation enhances the formation of non-bridging oxygen atoms. This leads to a decrease in the optical band gap energy. Radiation induced changes include hole trapping by bridging oxygen causing the increase of B–O bond length.

14/01605 Harvesting of oleaginous *Chlorella* sp. by organoclays

Lee, Y.-C. *et al. Bioresource Technology*, 2013, 132, 440–445.

In microalgae-based biorefinement, one of the highest practical priorities is to reduce the costs of downstream processes. As one potential solution, microalgae harvesting by organoclays has received particularly keen research interest. In the present study, cationic charged aluminium- and magnesium-backboned organoclays were synthesized and solubilized in aqueous solution due to their high-density of amino sites. Each, within 30 min of its injection into 1.7 g/L-concentration microalgal feedstocks, effected harvesting efficiencies of almost 100% at concentrations above 0.6 g/L while maintaining a neutral pH. Conclusively, organoclays, if recycled efficiently, can be uniquely effective microalgae harvesting agents.

14/01606 I-129 waste form using Bi-Zn-P-oxide glass

Yang, J. H. *et al. Energy Procedia*, 2013, 39, 151–158.

Iodine-129 is a problematic nuclide generated from the recycling of spent fuel by pyroprocess. The gaseous form of radiogenic iodine is trapped using silver-exchanged zeolite (AgX) at the Korea Atomic Energy Research Institute (KAERI). The authors developed the low-melting-temperature glass system based on Bi_2O_3-P_2O_5 composition. Various additives were included to modify the glass properties. It was found that ingots containing AgI are formed with ZnO, $CaCO_3$, MgO and Na_2CO_3 at around 600 °C. Analysis of microstructure and chemical durability revealed that AgI was encapsulated by a glass matrix and the formation of AgI compound is meaningful in fabricating iodine waste form.

14/01607 Studies of Ca-based high temperature sorbents for CO_2 capture

Arstad, B. *et al. Energy Procedia*, 2013, 37, 9–15.

Dolomite, a natural mineral, has been calcined and impregnated with Ti-, Zr-, Al-nanoparticle suspensions with the aim of improving the cyclic stabilities in high-temperature CO_2 sorption processes. After impregnation and subsequent calcination, the materials were characterized by N_2 adsorption (BET surface area and micropore volume) and powder X-ray diffraction (XRD) while the cyclic performance in CO_2 sorption processes was evaluated by breakthrough measurements: 30 cycles with sorption in 10% dry CO_2 at 600 °C and regeneration at 850 °C in N_2 were run on each sample. The XRD data showed that in addition to CaO and MgO, $CaTiO_3$, $CaZrO_3$ and $CaAl_2O_4$ are formed in respective synthesis. Breakthrough measurements show that the surface modified materials have less capacity (measured at 10% slip) compared to the calcined dolomite. However, the cyclic stability is satisfactory and the surface modification principle is likely to have some potential of improving natural sorbents.

14/01608 Super-adiabatic combustion in Al_2O_3 and SiC coated porous media for thermoelectric power conversion

Mueller, K. T. *et al. Energy*, 2013, 56, 108–116.

The combustion of ultra-lean fuel/air mixtures provides an efficient way to convert the chemical energy of hydrocarbons and low-calorific fuels into useful power. Matrix-stabilized porous medium combustion is an advanced technique in which a solid porous medium within the combustion chamber conducts heat from the hot gaseous products in the upstream direction to preheat incoming reactants. This heat recirculation extends the standard flammability limits, allowing the burning of ultra-lean and low-calorific fuel mixtures and resulting a combustion temperature higher than the thermodynamic equilibrium temperature of the mixture (i.e. super-adiabatic combustion). The heat generated by this combustion process can be converted into electricity with thermoelectric generators, which is the goal of this study. The design of a porous media burner coupled with a thermoelectric generator and its testing are presented. The combustion zone media was a highly porous alumina matrix interposed between upstream and downstream honeycomb structures with pore sizes smaller than the flame quenching distance, preventing the flame from propagating outside of the central section. Experimental results include temperature distributions inside the combustion chamber and across a thermoelectric generator; along with associated current, voltage and power output values. Measurements were obtained for a catalytically inert Al_2O_3 medium and a SiC-coated medium, which was tested for the ability to catalyse the super-adiabatic combustion. The combustion efficiency was obtained for stoichiometric and ultra-lean (near the lean flammability limit) mixtures of CH_4 and air.

14/01609 The effect of window shading design on occupant use of blinds and electric lighting

Sanati, L. and Utzinger, M. *Building and Environment*, 2013, 64, 67–76.

Occupant use of interior shading devices is one of the most influential factors in the admission of daylight into the buildings. Based on a number of observations, occupants do not adjust shading devices frequently, and once lowered, the blinds are left in place for days or even weeks leading to reduced energy savings from daylight. Previous shade control behaviour studies focus on environmental conditions such as transmitted vertical irradiance to predict the deployment of the shades; while there have been very few studies focusing on the factors that affect the raising of the interior shading devices by the occupants. This paper examines the effect of an interior lightshelf system on occupants' use of blinds and electric lighting. The results suggest that in identical environmental conditions, occupants whose workstations were located within the lightshelf zone demonstrated a lower window occlusion than those who were located in the area with conventional windows. Additionally, occupants in the lightshelf zone used less electric lighting than those in regular window design area.

14/01610 Utilization of boron oxide glass and epoxy/ilmenite assembly as two layer shield

Gaber, F. A. *et al. Annals of Nuclear Energy*, 2013, 57, 106–110.

This study considers the use of a boron oxide glass/epoxy ilmenite assembly (BOG/EI) as a two-layer shield. Experimental work regarding measurements of fast neutrons and gamma-ray leaking behind a homogenous and two-layer shield of BOG and EI composite have been carried out to investigate their radiation attenuation capabilities in terms of flux degradation. The measurements have been performed using a collimated beam emerging from spontaneous fission ^{252}Cf (100 μg) neutron source and the neutron-gamma spectrometer with stilbene organic scintillator based on the zero crossover method of the pulse shape discrimination technique. The MCNP-4C2 code was used to simulate the experimentally measured transmitted fast neutrons and gamma-ray fluxes theoretically for confirmation.

13 ALTERNATIVE ENERGY SUPPLIES

Biofuels and bioconversion energy

14/01611 A techno-economic assessment of biomass fuelled trigeneration system integrated with organic Rankine cycle

Huang, Y. *et al. Applied Thermal Engineering*, 2013, 53, (2), 325–331.

Biomass fuelled trigeneration is the term given to the system which is the on-site generation of electricity, heat and cooling simultaneously, using biomass as the fuel source. As a form of the renewable energy sources biomass is not intermittent, location-dependent or very difficult to store. If grown sustainably, biomass can be considered to be CO_2 neutral. Biomass, therefore, would be a promising option for the future to contribute both to the reduction of greenhouse gases and to the solution of replacing fossil fuels in power plants. For a wide range of commercial buildings, biomass trigeneration offers an economical solution of providing power, heat and cooling which is more environmentally friendly than conventional methods. This work

focuses on the modelling, simulation and techno-economic analysis of small-scale biomass trigeneration applications. The organic Rankine cycle (ORC) integrated with conventional combustion provides electricity for building use. The waste heat recovered from the ORC system and exhaust gases is used to supply hot water to space heating and excess heat is also used to drive an absorption cooling system. In order to use energy resources most efficiently, the proposed process is modelled and simulated using the ECLIPSE process simulation package. Based on the results achieved, the key technical and environmental issues have been examined. The study also investigates the impact of different biomass feedstock on the performance of trigeneration plant, biomass ash content ranges from 0.57 to 14.26% ash and a range of moisture content 10.6–33.51%. The calorific value across the biomass sources ranges between 16.56 and 17.97 MJ/kg daf. Finally, an economic evaluation of the system is performed along with sensitivity analyses such as capital investments, plant load factors and fuel costs. The results show that the maximum efficiencies and the best breakeven electricity selling price for the cases considered in this study are as follows: 11.1% and £221/MWh for power only, 85.0% and £87/MWh for combined heat and power and 71.7% and £103/kWh for trigeneration, respectively.

14/01612 Biogas utilization: experimental investigation on biogas flameless combustion in lab-scale furnace

Hosseini, S. E. and Wahid, M. A. *Energy Conversion and Management*, 2013, 74, 426–432.

Biogas generated in the anaerobic digestion of biomass and organic wastes by micro-organisms can be applied for heating, transportation and power generation as a renewable energy source. However, low calorific value (LCV) of biogas is one the most important bottlenecks of biogas conversion into electrical or thermal energy. Indeed, the presence of corrosive gases such as H_2S and water vapour in biogas components makes some dilemmas in biogas purification and utilization. In order to obtain the efficient biogas utilization method, different biogas resources, physical and chemical properties of biogas and biogas combustion characteristics should be considered. In this paper biogas was utilized in lab-scale flameless combustion furnace and the performance of flameless combustion chamber fuelled by biogas has been presented. Results demonstrated that flameless combustion is one of the best feasible strategies for biogas utilization. Uniformity of temperature in the flameless furnace increases the durability of refractory and related equipment. Simplicity of the flameless burner, pollutant formation reduction and fuel consumption decreases are the main causes of biogas flameless combustion supremacy.

14/01613 Brazilian biodiesel: the case of the palm's social projects

da Silva César, A. and Batalha, M. O. *Energy Policy*, 2013, 56, 165–174.

The Brazilian biodiesel programme (Programa Nacional de Produção e Uso do Biodiesel, PNPB) has created great demand for biodiesel. The production of oleaginous derived biodiesel produced by small-scale farmers is a key objective of the PNPB. The Social Fuel Seal is one of the instruments for achieving this goal. Five years after the mandatory implementation of programme, Brazil is among the world's leading producers of biodiesel. However, the goal of the productive insertion of small-scale farmers in Brazil's less-favoured regions has not been fully achieved. The Brazilian government has faced difficulties to promote regional development based on the PNPB, consequently not reaching the audacious goals that were set at the beginning of the programme. In this context of difficulties, the productive arrangements with palm oil should be emphasized. This paper considers the model developed by Agropalma – in partnership with public agencies – together with family farming in the north of Brazil. These social projects are taken as reference and can promote social inclusion in Brazil's national biodiesel productive chain. Moreover, this case can serve as an assessment tool for other countries that seek to invest in the production of biodiesel with the concern for the social production inclusion of disadvantaged small-scale family farmers.

14/01614 Catalytic upgrading of crude algal oil using platinum/gamma alumina in supercritical water

Duan, P. *et al. Fuel*, 2013, 109, 225–233.

This paper reports on the catalytic upgrading of crude oil, produced from the hydrothermal liquefaction of *Chlorella pyrenoidosa* over platinum on gamma alumina (Pt/γ-Al_2O_3) in supercritical water (SCW) at 400 °C for 1 h. The authors determined the influence of catalyst loading (varied from 0 to 40 wt%), water density (varied from 0 to 0.1 g/cm^3), and formic acid (HCOOH) loading (varied from 2 to 37 mmol) on the product yields and properties of the treated oil. The product yields and properties of the treated oil were largely insensitive to the catalyst loading and sensitive to water density and HCOOH loading. Increasing the catalyst loading or decreasing the water density and formic acid loading produced a lower yield but higher quality treated oil. Moreover, including the Pt/γ-Al_2O_3 in the reactor led to a product oil that was a freely flowing liquid, as opposed to being the viscous, sticky, and tar-like crude oil material. Compared to SCW + H_2, the presence of SCW + HCOOH effectively controls the coke formation. The catalyst experienced a reduction in surface area and micropore volume when used for hydrothermal upgrading. These changes did not influence the catalyst activity, however. Unreacted H_2 was the main gaseous product, together with lower yields of CO_2 and C_1–C_5 hydrocarbon.

14/01615 Changes in the Archaea microbial community when the biogas fermenters are fed with protein-rich substrates

Acs, N. *et al. Bioresource Technology*, 2013, 131, 121–127.

Terminal restriction fragment length polymorphism (T-RFLP) was applied to study the changes in the composition of the methanogens of biogas-producing microbial communities on adaptation to protein-rich monosubstrates such as casein and blood. Specially developed laboratory scale (5-L) continuously stirred tank reactors have been developed and used in these experiments. Sequencing of the appropriate T-RF fragments selected from a methanogen-specific (*mcrA* gene-based) library revealed that the methanogens responded to the unconventional substrates by changing the community structure. T-RFLP of the 16S rDNA gene confirmed the findings.

14/01616 Comparison of fuel and emission properties of petro diesel and sunflower biodiesel prepared by optimized production variables

Amini-Niaki, S. R. and Ghazanfari, A. *Fuel*, 2013, 109, 384–388.

Biodiesel is considered as a renewable fuel and an alternative to petro-diesel which is derived from transesterification of vegetable oils. In this research, the values of the major factors affecting the transesterification of sunflower oil were optimized by the response surface methodology. The experiments were conducted based on central composite rotatable design. A second-order polynomial model was developed for predicting biodiesel yield as a function of the dependent variables. The optimum values obtained for molar ratio of oil to methanol, the percentage of catalyst (KOH), reaction time and reaction temperature were 1 : 5.5, 1.0%, 65.5 min and 51.7 °C, respectively. The yield of biodiesel using the optimized variables was 83.4%. The fuel tests indicated that the prepared biodiesel had good combustion characteristics and lower exhaust pollutant in compare with regular petro-diesel.

14/01617 Culture of the hydrocarbon producing microalga *Botryococcus braunii* strain Showa: optimal CO_2, salinity, temperature, and irradiance conditions

Yoshimura, T. *et al. Bioresource Technology*, 2013, 133, 232–239.

Specific growth rates and hydrocarbon contents of *Botryococcus braunii* strain Showa were measured under a wide range of CO_2, salinity, temperature, and irradiance conditions. The bubbling CO_2 concentration of 0.2–5% and no addition of salinity were favourable conditions for growth. The strain cannot grow at 5 °C and above 35 °C under any irradiance levels. Maximum specific growth rate of 0.5 day^{-1} (doubling time of 1.4 days), the highest value reported for *B. braunii* in the past studies, was observed at 30 °C and 850 µmol photons m^{-2} s^{-1}. Since hydrocarbon productivity, shown as the product of hydrocarbon content and specific growth rate, increased with the increasing specific growth rate, it is concluded that more efficient hydrocarbon production by the mass culture of strain Showa can be achieved by maintaining higher specific growth rate based on the culture conditions presented in this study.

14/01618 Development of simplified anaerobic digestion models (SADM's) for studying anaerobic biodegradability and kinetics of complex biomass

Yusuf Momoh, O. L. *et al. Biochemical Engineering Journal*, 2013, 79, 84–93.

The anaerobic co-digestion of cow manure and waste paper at ambient temperature condition was observed to be optimized at a mix proportion of 75 : 25, respectively. The development and testing of a set of simplified anaerobic digestion models (SADMs) for this mixture revealed that the Hill-based biogas yield rate model was most appropriate in describing the kinetics of biogas production. Parameter estimation using non-linear regression analysis revealed that the half saturation constants expressed as acidified substrate and volatile solids equivalents were 0.228 g/L and 5.340 g VS/L, respectively. The maximum specific biogas yield rate and biodegradability were 2.2 mL/g VS/day and 0.313, respectively. The coefficients n and m, indicative of acidogenic bacterial adaptation for degradation and acetogenic/methanogenic bacterial cooperativity, were estimated to be 1.360 and 2.738, respectively. Hydrolysis/acidogenesis was considered the rate-limiting step. The need of bacterial adaptation may be an important factor to consider during anaerobic modelling of complex biomass.

14/01619 Emissions during co-firing of two energy crops in a PF pilot plant: cynara and poplar

Bartolomé, C. and Gil, A. *Fuel Processing Technology*, 2013, 113, 75–83.

Co-firing of coal and biomass appears as a promising technology to improve CO_2 emission levels. Even though it has been extensively studied, there is a need of widening the range of biomass fuels that could be applied to the process. With this aim, two energy crops (cynara and poplar) were tested with coal in a 500 kW_{th} co-firing pilot plant and compared from an emission viewpoint. Energy crops were co-fired with a bituminous coal at different shares (0–15%) in energy basis, and flue gas concentration (CO, CO_2, SO_2, O_2 and NO_x) was measured at stack. Combustion efficiency was evaluated by means of CO concentration, showing good performance in all cases and proving the feasibility of the process with low emissions. Small differences in particle size distribution are probably the main cause of different CO trends as cynara share is increased. SO_2 levels decreased for both cases, although, as expected, the SO_2 reduction was more pronounced for poplar co-firing than for cynara. NO_x emissions were higher in poplar experiments than in cynara mainly due to volatile matter content and air distribution differences. This work also includes a comparison with similar experimental results from literature, where high data variability was found.

14/01620 Enhancement of biodiesel production reaction employing the static mixing

Sungwornpatansakul, P. *et al. Fuel Processing Technology*, 2013, 116, 1–8.

Many reactors or mixers have been developed to enhance the reaction rate and reduce these requirements. In this research, a comparison of two mixing technologies, conventional mechanical mixer and the static mixer, was carried out. The conversion efficiency and kinetics show that the static mixer has a better performance. The static mixer has the potential to deliver better rigorous mixing between the raw oil and methanol, to the point that it can make the dispersed droplets of methanol in the raw oil smaller and more uniform, which resulted in enhancement of the reaction with the possibility of shortening the reaction time associated with biodiesel production.

14/01621 Evaluation of biodiesel production using lipase immobilized on magnetic silica nanocomposite particles of various structures

Kalantari, M. *et al. Biochemical Engineering Journal*, 2013, 79, 267–273.

Nonporous and mesoporous silica-coated magnetite cluster nanocomposites particles were fabricated with various silica structures in order to develop a desired carrier for the lipase immobilization and subsequent biodiesel production. Lipase from *Pseudomonas cepacia* was covalently bound to the amino-functionalized particles using glutaraldehyde as a coupling agent. The hybrid systems that were obtained exhibited high stability and easy recovery regardless of the silica structure, following the application of an external magnetic field. The immobilized lipases were then used as the recoverable biocatalyst in a transesterification reaction to convert the soybean oil to biodiesel with methanol. Enzyme immobilization led to higher stabilities and conversion values as compared to what was obtained by the free enzyme. Furthermore, the silica structure had a significant effect on stability and catalytic performance of immobilized enzymes. In examining the reusability of the biocatalysts, the immobilized lipases still retained approximately 55% of their initial conversion capability following five reuses.

14/01622 Experimental studies on spray and gas entrainment characteristics of biodiesel fuel: implications of gas entrained and fuel oxygen content on soot formation

Kuti, O. A. *et al. Energy*, 2013, 57, 434–442.

Experiments were performed inside the constant volume vessel to simulate the real diesel engine conditions. The LIF–PIV (laser-induced florescence – particulate image velocimetry) technique was used to characterize the spray and gas entrainment characteristics of the fuels while the OH-chemiluminescence and two-colour pyrometry were applied to obtain information about the combustion processes. Biodiesel from palm oil (biodiesel fuel, BDF) and the JIS #2 diesel fuel were utilized. It was observed that the Sauter mean diameter (SMD) obtained through an empirical equation decreased by increasing the injection pressure from 100 to 300 MPa and reducing the nozzle diameter from 0.16 to 0.08 mm. BDF has higher SMD values compared to diesel thus signifying inferior atomization. By increasing the injection pressure up to 300 MPa and reducing the nozzle diameter to 0.08 mm, the normal velocity and total mass flow rate of the entrained gas by the fuels increased. Due to higher viscosity and density properties, BDF possessed inferior atomization characteristics which made the normal velocity and total mass flow rate of the entrained gas lower compared to diesel. Due to inferior atomization which led to less gas being entrained upstream of the lift-off flame, the fuel oxygen content in BDF played a significant role in soot formation processes.

14/01623 γ-Alumina as a process advancing tool for a new generation biofuel

Syngiridis, K. *et al. Bioresource Technology*, 2013, 132, 45–48.

The production of volatile fatty acids (VFAs) in a continuous process using a synthetic glucose medium as model substrate in the presence of γ-alumina as promoter is described. The results showed formation of acetic, propionic, isobutyric, butyric, isovaleric and valeric acids, with acetic acid being more than 90% of the total VFAs produced. It is also highlighted that γ-alumina enhanced the simultaneous production of acetic acid and ethanol, which in some cases was formed at concentrations able to esterify about 85% of the produced VFAs. Since most agro-industrial effluents can be treated by anaerobic acidogenic digestion, while lignocellulosic biomass can be converted to VFAs after hydrolysis, this contribution can lead to a breakthrough in the research of biofuel production from renewable waste sources.

14/01624 Identification of *Monoraphidium contortum* as a promising species for liquid biofuel production

Bogen, C. *et al. Bioresource Technology*, 2013, 133, 622–626.

In this work, 30 microalgae strains from 17 genera were investigated in regard to biomass productivity in photoautotrophic growth conditions, lipid amount, lipid quality and biomass degradability. Six strains could be identified with robust phototrophic growth properties and high biomass productivities equal or above 300 $mg\,l^{-1}\,day^{-1}$. Anaerobic fermentation of the algal biomass was most efficient for the marine members of the genera *Dunaliella* and *Navicula*, while biogas production with the freshwater strains generally resulted in lower methane yields. *Monoraphidium contortum* was identified as promising candidate for liquid biofuel production, characterized by high biomass productivity during maximum growth (maximum increase of 896 mg dry biomass weight $l^{-1}\,day^{-1}$) and a promising lipid profile. Neutral lipid production was strongly induced in *M. contortum* by nitrogen deficient conditions and accumulated to up to $20.4 \pm 2.2\%$ of dry weight.

14/01625 Impact of various storage conditions on enzymatic activity, biomass components and conversion to ethanol yields from sorghum biomass used as a bioenergy crop

Rigdon, A. R. *et al. Bioresource Technology*, 2013, 132, 269–275.

With increased mandates for biofuel production in the USA, ethanol production from lignocellulosic substrates is burgeoning, highlighting the need for thorough examination of the biofuel production supply chain. This research focused on the impact storage has on biomass, particularly photoperiod-sensitive sorghum biomass. Biomass quality parameters were monitored and included biomass components, cellulose, hemicellulose and lignin, along with extra-cellular enzymatic activity (EEA) responsible for cellulose and hemicellulose degradation and conversion to ethanol yields. Analyses revealed dramatic decreases in uncovered treatments, specifically reduced dry matter content from 88% to 59.9%, cellulose content from 35.3% to 25%, hemicellulose content from 23.7% to 16.0% and ethanol production of 0.20 to 0.02 $g\,L^{-1}$ after 6 months of storage along with almost double EEA activities. In contrast, biomass components, EEA and ethanol yields remained relatively stable in covered treatments, indicating covering of biomass during storage is essential for optimal substrate retention and ethanol yields.

14/01626 In-depth investigation on the pyrolysis kinetics of raw biomass. Part I: kinetic analysis for the drying and devolatilization stages

Chen, D. *et al. Bioresource Technology*, 2013, 131, 40–46.

An in-depth investigation was conducted on the kinetic analysis of raw biomass using thermogravimetric analysis (TGA), from which the activation energy distribution of the whole pyrolysis process was obtained. Two different stages, namely, drying stage (stage I) and devolatilization stage (stage II), were shown in the pyrolysis process in which the activation energy values changed with conversion. The activation energy at low conversions (<0.15) in the drying stage ranged from 10 to 30 kJ/mol. Such energy was calculated using the non-isothermal Page model, known as the best model to describe the drying kinetics. Kinetic analysis was performed using the distributed activation energy model in a wide range of conversions (0.15–0.95) in the devolatilization stage. The activation energy first ranged from 178.23 to 245.58 kJ/mol and from 159.66 to 210.76 kJ/mol for corn straw and wheat straw, respectively, then increasing remarkably with an irregular trend.

14/01627 Microalgae-based carbohydrates for biofuel production

Chen, C.-Y. *et al. Biochemical Engineering Journal*, 2013, 78, 1–10.

Microalgae are considered as the most promising renewable feedstock for biofuel production and biorefineries, due to their advantages of fast growth, efficient carbon dioxide fixation, not competing for arable lands and potable water, and potentially accumulating high amounts of lipids and carbohydrates. Since carbohydrates in microalgae biomass are mainly cellulose in the cell wall and starch in the plastids without lignin and low hemicelluloses contents, they can be readily converted into fermentable sugars. However, to date there are very few studies focusing on the use of microalgae-based carbohydrates for biofuel production, which requires more understanding and knowledge to support the technical feasibility of this next-generation feedstock. This review article elucidates comprehensive information on the characteristics and metabolism of main fermentable microalgal carbohydrates (e.g. starch and cellulose), as well as the key factors and challenges that should be addressed during production and saccharification of microalgal carbohydrates. Furthermore, developments on the utilization of microalgae-based feedstock in producing liquid and gaseous biofuels are summarized. The understanding of the fundamentals underlying the carbohydrate metabolism of microalgae is a prerequisite for developing more effective strategies to increase the carbohydrates productivity, which should be optimized via manipulation of the key operating factors (such as light supply, nutrients starvation, temperature and carbon dioxide supplementation). In addition, more economic and effective saccharification processes should also be developed to enhance the efficiency of biofuel conversion through the microalgae biomass. To meet the demand of the biofuels market, large-scale processes for the cultivation of carbohydrates-rich microalgae should be developed with appropriate photobioreactor design. Moreover, economic assessment and life cycle analyses of the microalgae-based biofuels producing system should also be conducted to assess the commercial feasibility of converting microalgae-based carbohydrates into various biofuel products.

14/01628 Optimization of biodiesel production by supercritical methyl acetate

Goembira, F. and Saka, S. *Bioresource Technology*, 2013, 131, 47–52.

This work has been done to find out the optimum condition of supercritical methyl acetate method in biodiesel production. The reaction temperature, pressure, time and molar ratio in methyl acetate to oil were the key parameters that must be considered to produce an optimum condition. Evaluation of thermal decomposition on products, *cis–trans* isomerization and tocopherol content were required to further optimize the reaction condition. It was, therefore, concluded that for the supercritical methyl acetate method, reaction condition of 350 °C/20 MPa/45 min/42 M ratio gave the highest yields of FAME (96.7 wt%) and triacetin (8.8 wt%). Yet, at such a reaction condition, the optimum reaction condition was compromised due particularly to the unavoidable thermal decomposition of products, and tocopherols as natural anti-oxidants.

14/01629 Oxidation of hydrogen sulfide in biogas using dissolved oxygen in the extreme acidic biofiltration operation

Charnnok, B. *et al. Bioresource Technology*, 2013, 131, 492–499.

This work aimed to investigate the interactive effects of empty bed retention time (*EBRT*), specific hydraulic loading rate (q) and initial pH (pH_i) of the aerated recirculating liquid to remove H_2S in extreme acidic biofiltration. Biogas containing H_2S 6395 ± 2309 ppm and CH_4 $79.8 \pm 2.5\%$ was fed to the biofilter as pH of the high dissolved oxygen recirculating liquid swung between pH_i to 0.5. Response surface methodology was employed that gave the H_2S removal relationship model with R^2 0.882. The predicted highest H_2S removal within the studied parameter ranges was 94.7% at *EBRT* 180.0 s, q 4.0 $m^3/m^2/h$ and pH_i 3.99. Results from separate runs at a random condition were not statistically different from the model prediction, signifying a validity of the model. Additionally, CH_4 content in the exit biogas increased by $4.7 \pm 0.4\%$. *Acidithiobacullus* sp. predominance in the consortia of this extreme acidic condition was confirmed by DGGE.

14/01630 Oxidative stability of biodiesels produced from vegetable oils having different degrees of unsaturation

Pantoja, S. S. *et al. Energy Conversion and Management*, 2013, 74, 293–298.

In this study, methyl esters were obtained from the transesterification of cupuaçu fat lipids (*Theobroma grandiflorum*) (Willd. ex Spreng.) (K. Schum.), açaí (*Euterpe oleracea*), passion fruit (*Passiflora edulis*) and linseed (*Linum usitatissimum* L.) oils, using a basic catalyst. The triglycerides were characterized by their fatty acid composition, and the biodiesels were characterized according to standard methods. The critical properties, such as the cold filter plugging point, kinematic viscosity and oxidative stability, of the biodiesels were studied. The influence of butyl-hydroxyanisole, propyl gallate and tert-butyl hydroquinone antioxidants on the acaí, passion fruit and linseed biodiesels was evaluated at concentrations from 500 to 4000 ppm. Propyl gallate was found to be the most efficient antioxidant for the studied biodiesels.

14/01631 Production of biodiesel fuel by transesterification of different vegetable oils with methanol using Al_2O_3 modified MgZnO catalyst

Olutoye, M. A. and Hameed, B. H. *Bioresource Technology*, 2013, 132, 103–108.

An active heterogeneous Al_2O_3 modified MgZnO (MgZnAlO) catalyst was prepared and the catalytic activity was investigated for the transesterification of different vegetable oils (refined palm oil, waste cooking palm oil, palm kernel oil and coconut oil) with methanol to produce biodiesel. The catalyst was characterized by using X-ray diffraction, Fourier transform infrared spectra, thermo gravimetric and differential thermal analysis to ascertain its versatility. Effects of important reaction parameters such as methanol to oil molar ratio, catalyst dosage, reaction temperature and reaction time on oil conversion were examined. Within the range of studied variability, the suitable transesterification conditions (methanol/oil ratio 16 : 1, catalyst loading 3.32 wt%, reaction time 6 h, temperature 182 °C), the oil conversion of 98% could be achieved with reference to coconut oil in a single stage. The catalyst can be easily recovered and reused for five cycles without significant deactivation.

14/01632 Regional differences in the economic feasibility of advanced biorefineries: fast pyrolysis and hydroprocessing

Brown, T. R. *et al. Energy Policy*, 2013, 57, 234–243.

This analysis identifies the sensitivity of the fast pyrolysis and hydroprocessing pathway to facility location. The economic feasibility of a 2000 metric tons per day fast pyrolysis and hydroprocessing biorefinery is quantified based on 30 different state-specific facility locations within the USA. The authors calculate the 20-year internal rate of return (IRR) and net present value (NPV) for each location scenario as a function of state- and region-specific factors. This analysis demonstrates that biorefinery IRR and NPV are very sensitive to bio-oil yield, feedstock cost, location capital cost factor, and transportation fuel market value. The IRRs and NPVs generated for each scenario vary widely as a result, ranging from a low of 7.4% and −$79.5 million in Illinois to a high of 17.2% and $165.5 million in Georgia. The results indicate that the economic feasibility of the fast pyrolysis and hydroprocessing pathway is strongly influenced by facility location within the United States. This result could have important implications for cellulosic biofuel commercialization under the revised renewable fuel standard.

14/01633 Revising the potential of large-scale Jatropha oil production in Tanzania: an economic land evaluation assessment

Segerstedt, A. and Bobert, J. *Energy Policy*, 2013, 57, 491–505.

Following up the rather sobering results of the biofuels boom in Tanzania, this study analyses the preconditions that would make large-scale oil production from the feedstock *Jatropha curcas* viable. The authors do this by employing an economic land evaluation approach; first, they estimate the physical land suitability and the necessary inputs to reach certain amounts of yields. Subsequently, they estimate costs and benefits for different input-output levels. Finally, to incorporate the increased awareness of sustainability in the export sector, the authors introduce certification criteria. Using data from an experimental farm in Kilosa, they found that high yields are crucial for the economic feasibility and that they can only be obtained on good soils at high input rates. Costs of compliance with certification criteria depend on site specific characteristics such as land suitability and precipitation. In general, both domestic production and (certified) exports are too expensive to be able to compete with conventional diesel/rapeseed oil from the European Union. Even though the crop may have potential for large-scale production as a niche product, there is still a lot of risk involved and more experimental research is needed.

14/01634 Small-scale storage techniques for fuel chips from short rotation forestry

Manzone, M. *et al. Fuel*, 2013, 109, 687–692.

The experiment determined the technical and financial efficiency of five storage techniques, specifically designed for short rotation forestry poplar chips stored at the farm site in small (20 m^3) piles. The treatments on test were: uncovered storage, storage under a temporary roof structure, cover under a semi-permeable fleece sheet, cover under two types of plastic sheet (i.e. white and black). Each treatment was replicated three times. Researchers monitored temperature and moisture content trends inside the piles, and determined dry matter losses at the end of the 170 days storage period. In general, piles under plastic cover presented opposite trends compared to all other piles. They acquired moisture rather than losing it, and showed gradual temperature trends instead of a typical peak-and-drop behaviour. Dry

matter losses varied from 5.1% to 9.8%, and were highest for the uncovered treatment, and lowest for the plastic cover treatment. Under the conditions of north-western Italy, uncovered storage was a cost-effective option. Protecting the piles with some cover incurred more cost than it saved, resulting in a higher storage cost per unit energy. Although more expensive, sheltering the piles under a simple roof structure offered the benefit of a higher reduction of moisture content, which may turn the chips into a higher quality fuel. Of course, these results were closely related to the southern European climate, and the specific year of the test. Occasional wetter years may overturn these results.

14/01635 Software sensors design for the simultaneous saccharification and fermentation of starch to ethanol

López Pérez, P. A. *et al. Fuel*, 2013, 110, 219–226.

A local analysis of stability and observability of the ethanol process were determined for continuous operation. It was found that the process is stable and non-completely observable in the selected steady states. The analysis of observability was studied in terms of the observability matrix rank conditions. Furthermore, the authors designed a non-linear observer in order to estimate the observable state variables. The software sensor (state estimator) was developed considering only one measurable variable, the glucose concentration, and taking in account model uncertainties, which is a realistic issue. Some sufficient conditions for the existence of the proposed observer were obtained, which guarantee the convergence of the proposed methodology. The maximum ethanol production conditions were obtained by manipulating the dilution rate with optimal initial substrate concentration and the observable subspace was determinate which allows estimating six state variables (starch concentration, susceptible starch concentration, ethanol concentration, biomass concentration, glucose concentration and enzyme concentration). Numerical simulations were provided to show the effectiveness of the proposed observer where a comparison with a standard sliding-mode observer was carried out.

14/01636 Spatial variation of chemical constituents from the burning of commonly used biomass fuels in rural areas of the Indo-Gangetic Plain (IGP), India

Saud, T. *et al. Atmospheric Environment*, 2013, 71, 158–169.

This study determined the emission factor of chemical composition of the emission from the burning of biomass (e.g. Dung cake, *Acacia*, *Neem*, *Mulberry*, *Indian Rosewood*, *Pigeon pea*, etc.) commonly used as a residential fuel in the rural sector of Indo-Gangetic Plain (IGP) (Delhi, Punjab, Haryana, Uttar Pradesh, Bihar and West Bengal), India. For comparison, the authors have selected only those biomass fuels, which are used in at least three of the above-mentioned states. Dung cake from all the states reports highest emission of particulate matter (PM) (15.68 $g\,kg^{-1}$), organic carbon (OC) (4.32 $g\,kg^{-1}$) and elemental carbon (EC) (0.51 $g\,kg^{-1}$). Among all biomass fuels studied, agricultural residue reports substantial amount of emission of Na^+ (104 $mg\,kg^{-1}$), K^+ (331 $mg\,kg^{-1}$) and Cl^- (447 $mg\,kg^{-1}$) particularly in *Pigeon pea* and Mustard stem. Eucalyptus (fuel wood) emits large amounts of Ca^{2+} (21.47 $mg\,kg^{-1}$) and NO_3^- (614 $mg\,kg^{-1}$). The emission of PM from dung cake is higher in Delhi (19.31 $g\,kg^{-1}$) and followed by Uttar Pradesh (17.58 $g\,kg^{-1}$) > Haryana (15.46 $g\,kg^{-1}$) > Bihar (14.99 $g\,kg^{-1}$) > Punjab (12.06 $g\,kg^{-1}$) > West Bengal (5.90 $g\,kg^{-1}$). Carbonaceous aerosols (OC and EC) and dominant ionic species (Cl^-, K^+, SO_4^{2-}, NO_3^- and PO_4^{3-}) are altogether contributing 40–70% of total emissions. Characteristics and ratios of chemical species of emissions may help to develop a methodology of discriminating the sources of ambient particulate matter. Using a laboratory determined emission factor of chemical species, the authors have determined the emission budget over IGP, India.

14/01637 Synthesis gas production through biomass direct chemical looping conversion with natural hematite as an oxygen carrier

Huang, Z. *et al. Bioresource Technology*, 2013, 132, 138–145.

Biomass direct chemical looping (BDCL) conversion with natural hematite as an oxygen carrier was conducted in a fluidized bed reactor under argon atmosphere focusing on investigation the cyclic performance of oxygen carrier. The presence of oxygen carrier can evidently promote the biomass conversion. The gas yield and carbon conversion increased from 0.75 $N\,m^3/kg$ and 62.23% of biomass pyrolysis to 1.06 $N\,m^3/kg$ and 87.63% of BDCL, respectively. The components of the gas product in BDCL were close to those in biomass pyrolysis as the cyclic number increased. The gas yield and carbon conversion decreased from 1.06 $N\,m^3/kg$ and 87.63% at first cycle to 0.93 $N\,m^3/kg$ and 77.18% at twentieth cycle, respectively, due to the attrition and structural changes of oxygen carrier. X-ray diffraction analysis showed that the reduction extent of oxygen carrier increased with the cycles. Scanning electron microscope and pore structural analysis displayed that agglomeration was observed with the cycles.

14/01638 Techno-economic assessment of carbon-negative algal biodiesel for transport solutions

Taylor, B. *et al. Applied Energy*, 2013, 106, 262–274.

This paper presents a techno-economic analysis of carbon-negative algal biodiesel production routes that use currently available technologies. The production process includes the following stages: carbon-neutral renewable electricity generation for powering the plant, algal growth in photobioreactors, algae dewatering and lipid extraction, and biofuel conversion and refining. As carbon dioxide is consumed in the algal growth process, side products are not burned (with CO_2 release), and the energy supplied to the entire production process is obtained from concentrated solar power, the whole system is assumed to have a negative carbon footprint. Under assumptions related to economics of scale, the techno-economic model is extended to account for varying industrial scales of production. Verified data from a selection of commercially available technologies are used as inputs for the model, and the economic viability of the various production routes is assessed. From the various routes investigated, one scheme involving combined gasification and Fischer–Tropsch of algal solids to produce biodiesel along with conversion of algal lipids into biodiesel through transesterification was found to be promising. Assuming a typical economic scaling factor of 0.8, an algal biodiesel process with an annual production rate of 100 Mt/year is identified to achieve a biodiesel price comparable to the current conventional diesel price (approximately £1.39/litre at the pump, or $114/barrel of crude) with a discounted break-even time of 6 years.

14/01639 Technoeconomic assessment of potential processes for bio-ethylene production

Haro, P. *et al. Fuel Processing Technology*, 2013, 114, 35–48.

The use of biomass in the production of plastics can contribute to the depletion of greenhouse gas emissions and secondarily to partially fulfill the growing demand for plastics expected in the near future. The aim of this study is to assess the production of ethylene, one of the most important commodities in the petrochemical industry, via the dehydration of bioethanol and the conversion of bio-dimethyl ether (bio-DME) into olefins. Four case studies have been developed taking into account the different origins of bioethanol, and one for the conversion of bio-DME. The assessment includes current and promising processes for the production of bioethanol, i.e. first- and second-generation bioethanol. The latter comprises biochemical processing (enzymatic hydrolysis), thermochemical processing (both direct and indirect syntheses from syngas) and hybrid processing (fermentation of syngas) of biomass. The results show that two of the considered case studies (Brazilian ethanol and ethanol via indirect synthesis from syngas) enable the cost-competitive production of ethylene at current market prices. If bioenergy with carbon capture and storage is taken into account for the case studies, the results would be substantially enhanced and all cases, except for the case of bioethanol from biochemical processing, would be profitable.

14/01640 The applicability of the renewable energy directive calculation to assess the sustainability of biogas production

Manninen, K. *et al. Energy Policy*, 2013, 56, 549–557.

Biogas production processes are often multifunctional systems, which also produce fertilizers from digested sludge. The environmental impacts of such systems are usually determined using life cycle assessment (LCA). There are alternative approaches to conduct the LCA, e.g. allocation of emissions based on a product's and co-product's energy content according to the renewable energy directive (RED), or substitution without allocation according to the ISO 14040 standard. The authors calculated the climate change impacts of biogas production using these two alternative methods, while also considering process modifications of the base case biogas production process. The aim was to find out whether the production system achieves the saving targets for greenhouse gas emissions set by the RED. Since the RED enables different interpretations of its calculation rules, four case studies were created representing alternative ways to allocate the emissions to the reject water and solid fractions separated from the sludge. Consequently, the emission estimates for the base case vary between 16.9 and 47.7 g CO_2/MJ, while the emission savings range from 42% to 80%. Most of the case studies achieved the most stringent saving target (60%).

14/01641 The optimization of biodiesel production by using response surface methodology and its effect on compression ignition engine

Abuhabaya, A. *et al. Fuel Processing Technology*, 2013, 113, 57–62.

Biofuel production provides an alternative non-fossil fuel without the need to redesign current engine technology. This study presents an experimental investigation into the effects of using biodiesel blends on diesel engine performance and its emissions. The biodiesel fuels were produced from sunflower oil using the transesterification process with low molecular weight alcohols and sodium hydroxide then tested on a

steady state engine test rig using a Euro 4 four-cylinder compression ignition engine. This study also shows how by blending biodiesel with diesel fuel at intervals of B5, B10, B15 and B20 can decrease harmful gas emissions significantly while maintaining similar performance output and efficiency. Production optimization was achieved by changing the variables which included methanol/oil molar ratio, NaOH catalyst concentration, reaction time, reaction temperature, and the rate of mixing to maximize biodiesel yield. The technique used was the response surface methodology. In addition, a second-order model was developed to predict the biodiesel yield if the production criteria is known. The model was validated using additional experimental testing. It was determined that the catalyst concentration and molar ratio of methanol to sunflower oil were the most influential variables affecting percentage conversion to fuel and percentage initial absorbance.

14/01642 Thermal behavior of renewable diesel from sugar cane, biodiesel, fossil diesel and their blends

Conconi, C. C. and Crnkovic, P. M. *Fuel Processing Technology*, 2013, 114, 6–11.

Biofuels and their blends with fossil fuel are important energy resources, whose production and application have been largely increased internationally. This study focuses on the evaluation of the activation energy of the thermal decomposition of three pure fuels: farnesane (renewable diesel from sugar cane), biodiesel and fossil diesel and their blends (20% farnesene and 80% of fossil diesel – 20F80D and 20% farnesane, 50% fossil diesel and 30% biodiesel – 20F50D30B). Activation energy has been determined from thermogravimetry and model-free kinetics. Results showed that not only the cetane number is important to understand the behaviour of the fuels regarding ignition delay, but also the profile of the activation energy versus conversion curves shows that the chemical reactions are responsible for the performance at the beginning of the process. In addition, activation energy seemed to be suitable in describing reactivity in the case of blends of renewable and fossil fuels.

14/01643 Thermo-chemical conversion of *Chlorella pyrenoidosa* to liquid biofuels

Duan, P. *et al. Bioresource Technology*, 2013, 133, 197–205.

This study considered how the solvent polarity affects the liquefaction behaviour of *Chlorella pyrenoidosa* and subsequently, using the most suitable solvent identified, explored effect of solvent/biomass ratio, time, and temperature on the product yield and properties of the bio-oil. The product yield was significantly affected by the solvent type, and ethanol was proven to be the most suitable solvent to convert *C. pyrenoidosa* into bio-oil from the yield and economic points of view. Temperature is the most influential factor on the products yield and properties of the bio-oil. The higher heating values of the bio-oils produced under different reaction conditions are within the range of 27.68–36.45 MJ/kg. The major compounds in bio-oil were esters, fatty acids, alkenes, aldehydes, and amides, and fatty acid ethyl esters were the largest portion.

14/01644 Transient behavior of devolatilization and char reaction during steam gasification of biomass

Moon, J. *et al. Bioresource Technology*, 2013, 133, 429–436.

Steam gasification of biomass is a promising method for producing high quality syngas for polygeneration. During the steam gasification, devolatilization and char reaction are key steps of syngas production and the contributions of the two reactions are highly related to gasification conditions. In this study, the transient characteristics of devolatilization and char reaction in biomass steam gasification were investigated by monitoring cumulative gas production and composition changes in terms of reaction temperature and S/B ratio. Contribution of each reaction stage on the product gas yield was studied in detail. The results provide important insight for understanding the complex nature of biomass gasification and will guide future improvements to the biomass gasification process.

14/01645 Using solar energy to enhance biogas production from livestock residue – a case study of the Tongren biogas engineering pig farm in South China

Dong, F. and Lu, J. *Energy*, 2013, 57, 759–765.

Due to the rapid growth in the global energy demand and to the growing concerns regarding energy supply, more attention has been paid to the development of bioenergy, especially the one derived from anaerobic digestion. The study used solar energy to improve the efficiency of anaerobic fermentation at the Tongren pig farm in Haining city, Zhejiang province, China. Haining, located at 30°15′–30°35′N and 120°18′–120°52′E, has the average winter temperature of about 5 °C. At the farm, solar energy collectors, with a total area of 100.8 m^2 and a volume of 6 t water were installed to heat the water in fermentation digesters. Comparison shows that biogas production was 2540 m^3 more or 11.2% higher than that of the CK with no differences in the methane content, which can also be translated into a 14.3% increase of pig manure energy transformation efficiency.

Geothermal energy

14/01646 Borehole thermal response and thermal resistance of four different grouting materials measured with a TRT

Borinaga-Treviño, R. *et al. Applied Thermal Engineering*, 2013, 53, (1), 13–20.

Among other systems, closed-loop geothermal heat exchangers are extensively used due to the lower environmental impact compared to open-loop systems. Thermal conductivity is the main parameter required for the design of the geothermal heat exchangers, which is determined by the thermal response test (TRT). However, in most of the design cases only one TRT is done per project because of its cost. Therefore, there is no available data to contrast with the measured ones and the data obtained must be taken as valid. Four different TRTs are executed in four different boreholes to analyse the reliability of the estimated thermal conductivity. Each of the boreholes tested has similar geological and geometric characteristics, but the grouting material is different in each of them. Basic oxygen furnace (G_2), silica sand (G_3) and construction and demolition waste (G_4) have been used as base aggregates in cement based self-compacting mortars, and compared with a cement–bentonite–graphite (G_1) grouting material. Results indicate that thermal conductivity of the ground is between 2.2 and 2.58 W/(m K). However, this value is influenced by the water content of the ground during the performance of the test. According to the borehole thermal resistance (R_b), the G_1 mix performs the best, but G_4 has similar values. Laboratory measured grout thermal conductivity has not been a good estimation parameter for the determination of the R_b, since contact resistance between the pipes and the grout is of importance due to the shrinkage of the cement based mixes.

14/01647 Energetic and economic evaluations of geothermal district heating systems by using ANN

Keçebaş, A. *et al. Energy Policy*, 2013, 56, 558–567.

This paper proposes an artificial neural network (ANN) technique as a new approach to evaluate the energy input, losses, output, efficiency and economic optimization of a geothermal district heating system (GDHS). By using ANN, an energetic analysis is evaluated on the Afyon geothermal district heating system (AGDHS) located in the city of Afyonkarahisar, Turkey. Promising results are obtained about the economic evaluation of that system. This has been used to determine if the existing system is operating at its optimal level, and will provide information about the optimal design and profitable operation of the system. The results of the study show that the ANN model used for the prediction of the energy performance of the AGDHS has good statistical performance values: a correlation coefficient of 0.9983 with minimum root mean square and mean absolute percentage error values. The total cost for the AGDHS is profitable when the PWF is higher than 7.9. However, the present worth factor (PWF) of the AGDHS was found to be 1.43 for the given values. As a result, while installing a GDHS, one should take into account the influences of the PWF, ambient temperature and flow rate on the total costs of the system in any location where it is to be established.

14/01648 Experimental and CFD simulation of heat efficiency improvement in geothermal spas

Jalilinasrabady, S. *et al. Energy*, 2013, 56, 124–134.

Hot spas and jacuzzis are popular in Iceland due to the abundance of reasonably prized geothermal heat available. However, water from the district heating (DH) system is too warm to be admitted directly into the spa. For safety reasons the water is mixed with cold water, from 75 °C down to 50 °C, which leads to the waste of a large quantity of heat. Therefore, a design was suggested that enables the feeding of geothermal water directly into the pot, omitting the step of mixing it with cold water. The idea is to employ an open heat exchanger that transfers heat from the geothermal water to the bulk water in the spa, before letting it mix with the spa water. A case study was done for one particular spa. Heat load was calculated and measured when the spa was in use, and when it was unused. A design is suggested employing a circular double-plate which is to be placed at the bottom of the pot. This unit will function as an open heat exchanger feeding DH water into the pot. Free convection takes place at the up side of the upper plate and forced convection below the upper plate. Heat-transfer coefficient for both was calculated. Temperature field in the pool before and after implementation of the open heat exchanger was measured at different points using thermocouples. The measured temperatures were compared to thermal and fluid-dynamic simulation of the temperature and flow fields obtaining good accordance. Results are reasonable and promising for a good design that may considerably reduce the energy expenses for a continuously heated geothermal spa. More detailed measurements were made on the upper plate of the heat exchanger and detailed simulation of the heat exchanger itself was then used to obtain a value for the heat-transfer coefficient for the upper

plate to the surrounding water. This information was used to make an improved design for the open plate heat exchanger, stating that a diameter of 63 cm and a thickness of 1.5 cm were suggested as final design. Due to economy consideration the recovery time of the implementing of suggested heat exchanger is estimated to 8 months in the studied case.

14/01649 Ground thermal conductivity for (ground source heat pumps) GSHPs in Korea

Shim, B. O. and Park, C.-H. *Energy*, 2013, 56, 167–174.

The aim of this study is to evaluate the characteristic thermal properties of 208 thermal response test (TRT) data sets collected in Korea. In the evaluation, the line-source model is used in conjunction with the step-wise evaluation to validate the applicability of the model. The applicability of the step-wise evaluation is classified focusing on the convergence criterion of ground thermal conductivities. The ground thermal conductivities were evaluated in the range of 1.73 and 8.56 W/m·K with the mean of 2.55 W/m·K. The corresponding borehole thermal resistances were also obtained in the range between 0.06 and 0.20 m·K/W with the mean 0.13 m·K/W. In order to investigate the availability of the thermal conductivity of the test sites from the geothermal database in Korea, the ground thermal conductivity obtained by TRTs was compared with the mean bedrock thermal conductivity. Comparison of the four major bedrocks in the test sites indicated that the mean differences are 0.34, 0.53, 0.22 and 1.39 W/m·K at the bedrocks of the granite, geneiss, tuff and sandstone areas, respectively.

14/01650 Numerical simulation of heat production potential from hot dry rock by water circulating through two horizontal wells at Desert Peak geothermal field

Zeng, Y.-C. *et al. Energy*, 2013, 56, 92–107.

In this work, heat production potential from hot dry rock by water circulating through two horizontal wells was numerically investigated based on the geological data of well DP23–1 under the enhanced geothermal system project at Desert Peak geothermal field. The results indicate that the desirable electricity production power and energy efficiency can be obtained under suitable reservoir permeability, water production rate and injection temperature; meanwhile water flow impedance remains at a relative lower level. The sensitivity analysis indicates that the electricity production power mainly depends on the water production rate and the injection temperature; the water flow impedance mainly depends on the reservoir permeability, water production rate and injection temperature; the energy efficiency mainly depends on the reservoir permeability and the water production rate. The heat production performance will be improved when the reservoir permeability, the water production rate and the injection temperature are under reasonable conditions. However, this study is based on that the fractured reservoir is equivalent to a homogeneous porous medium and there is no water loss in the reservoir, so the practical energy output and efficiency of water circulating through two horizontal wells at Desert Peak geothermal field needs further study in the future.

14/01651 Performance evaluation of Kalina cycle subsystem on geothermal power generation in the oilfield

Fu, W. *et al. Applied Thermal Engineering*, 2013, 54, (2), 497–506.

Geothermal energy resource of oilfield can be used to generate electricity in the high water-cut period. A cascade utilization system including Kalina cycle (KC) subsystem and oil production process subsystem is proposed. A model of the Kalina cycle subsystem is calculated numerically and validated. The KC subsystem is optimized by analysing the thermal and exergetic efficiencies. The feasibility of removing the low-temperature (LT) recuperator and the turbine protection are then analysed, respectively. Finally, the economic performance of the cascade utilization system is evaluated. Results show that the ammonia concentration and the inlet pressure of the turbine should be lower than that of the optimum points in order to ensure the system stability. The LT recuperator is not necessary for high condensation temperature. Lower ammonia concentration and higher pressure result in higher liquid amount at the turbine outlet. The economic benefits of the power plant in the oilfield are great and the total rewards of the crude oil and the power generation can reach US$2 million per year.

14/01652 Thermal enhancement of PFA-based grout for geothermal heat exchangers

Alrtimi, A. A. *et al. Applied Thermal Engineering*, 2013, 54, (2), 559–564.

As part of a programme of finding new uses for industrial wastes, a trial of PFA (pulverized fuel ash) as a thermal grout for borehole heat exchangers has been tested experimentally. Several mixes of PFA-based grouts were developed by blending PFA with different solid materials by weight in different mix proportions with a constant percentage of cement. The materials used in these mixes are: fine sand, coarse sand, ground glass, and fluorspar. The thermal conductivity of seven different groups of grouts has been measured at dry and saturated conditions. A new thermal cell that utilizes the steady state technique developed by Newcastle University was used for these measurements. The results show poor enhancement of thermal conductivity using fine sand or medium ground glass, with maximum value of 1.15 W/m K at saturation. Results obtained using coarse or mixed ground glass gave a maximum value of 1.39 W/m K. The highest thermal conductivity values were achieved using fluorspar or coarse sand where the thermal conductivity reached 2.88 and 2.47 W/m K respectively at 20% of PFA. It was also observed that the combination of fluorspar with coarse ground glass can offer relatively high thermal conductivity at both dry and saturated conditions. Moreover, this combination of materials comprises a practical amount of low-cost material (PFA and ground glass).

14/01653 Utilization of carbon dioxide from coal-based power plants as a heat transfer fluid for electricity generation in enhanced geothermal systems (EGS)

Mohan, A. R. *et al. Energy*, 2013, 57, 505–512.

The feasibility of using CO_2 as a heat transfer fluid by organic Rankine cycle (ORC) in enhanced geothermal systems (EGS) in arid regions is explored in this paper. As CO_2 is available for sequestration at high pressures from an integrated gasification combined cycle (IGCC) plant, this idea is examined by pairing an IGCC plant with an EGS plant to facilitate both the simultaneous extraction of geothermal heat and sequestration of CO_2 as well as power generation from EGS. The ORC portion of EGS was modelled by ASPEN Plus version 7.3. Four different working fluids were chosen for the ORC portion of the EGS to absorb the geothermal energy from the CO_2 in a binary heat exchanger. The power generated from the EGS and the lowest possible temperature at which CO_2 can be discharged from the binary heat exchanger was evaluated for each working fluid. The addition of a preheater provides an opportunity to add a second cycle so that both CO_2 and the working fluid can be discharged at the lowest possible temperature. In all cases, the thermal energy recovered from the EGS reservoir is substantially higher than that required to compress the CO_2 stream from the IGCC for sequestration.

Solar energy

14/01654 A counter electrode of multi-wall carbon nanotubes decorated with tungsten sulfide used in dye-sensitized solar cells

Yue, G. *et al. Carbon*, 2013, 55, 1–9.

Multi-wall carbon nanotubes decorated with tungsten sulfide (MWCNTs-WS_2) were synthesized by using a hydrothermal method, and used as a low-cost platinum-free counter electrode for dye-sensitized solar cell (DSSC). Cyclic voltammetry and electrochemical impedance spectroscopy characterizations indicate that the counter electrode has a high catalytic activity for the reduction of triiodide to iodide and a low charge transfer resistance at the electrolyte–electrode interface. A DSSC based on this counter electrode achieves a high power conversion efficiency of 6.41% under a simulated solar illumination of 100 mW cm^{-2} (AM 1.5). This efficiency is comparable to 6.56% for a DSSC with Pt counter electrode.

14/01655 Effects of a cut-off in feed-in tariffs on photovoltaic capacity: evidence from Germany

Leepa, C. and Unfried, M. *Energy Policy*, 2013, 56, 536–542.

This study analyses the effects of feed-in tariff (FIT) adjustments on installed photovoltaic capacity in Germany. It was found that the current system temporarily accelerates instalments and does not nullify over-investment. Therefore, three alternative FIT regimes were designed: (i) constant FITs, (ii) linearly decreasing FITs and (iii) FIT adjustments related to the changes of photovoltaic panel prices. Simulations of installed capacities indicate that alternative adjustment mechanisms could be more appropriate to meet the government's installation target. Moreover, the consumers' burden induced by the FITs was calculated and it was found that it might be reduced by alternative mechanisms.

14/01656 Effects of solar shading devices on energy requirements of standalone office buildings for Italian climates

Bellia, L. *et al. Applied Thermal Engineering*, 2013, 54, (1), 190–201.

In Europe, the building energy demand is about 40% of the total energy requirement. In order to obtain significant energy saving in this sector, the European Energy Performance Building Directive (EPBD) 2002/91/CE and the EPBD Recast (Directive 2010/31/UE) promote the use of passive strategies for buildings, which improve indoor thermal

conditions above all in summer and so allow the reduction of size and energy requirements of air conditioning systems. This paper analyses the influence of external solar shading devices on the energy requirements of a typical air-conditioned office building for Italian climates. A type of office building widespread in Europe has been considered. The energy saving related to the solar shading refers only to summer air conditioning, but the evaluation has been carried out for the entire year, by using a building energy simulation code. The energy demand of the main technical systems (heating, cooling and lighting) and the energy saving related to the use of solar shading devices have been evaluated, as a function of the most significant parameters, such as the climate, the geometrical characteristics of the shadings and the building, the thermal transmittance of the building envelope and the building orientation. The solar shading devices have shown the highest energy efficiency for warm summer climates: for example, the global annual energy saving related to the use of suitable shading devices has been evaluated between 8% for Milan (the coldest climate) and 20% (for Palermo, the warmest one).

14/01657 Experimental analysis of the effectiveness of a high temperature thermal storage tank for solar cooling applications

Gil, A. *et al. Applied Thermal Engineering*, 2013, 54, (2), 521–527.

Thermal energy storage (TES) systems are growing to a relevant role in solar cooling applications. Hence, high energy density is a desirable property of the TES system. Phase change materials (PCM) helps to increase this characteristic. A high temperature pilot plant able to test different types of TES systems and materials was designed and built at the University of Lleida in Spain. This pilot plant is composed mainly of three parts: heating system, cooling system, and different storage tanks. Two identical storage tanks based on the shell-and-tubes heat exchanger, one of them including 196 squared fins in the bundle of the tubes and the other without, were experimentally tested. Hydroquinone was selected as the storage material, having a latent heat of 205 kJ/kg and a phase change temperature between 168 and 173 °C. The aim of this paper is to test experimentally, and compare the average effectiveness of the TES systems analysed using PCM for solar cooling and refrigeration applications. It was found out that for the same tank configurations (shell-and-tubes) even changing drastically the dimensions of the tank or the number and the diameter of the tubes, the average effectiveness curve proposed in the literature fits well with the results showed here.

14/01658 Experimental verification of PV based dynamic voltage restorer (PV-DVR) with significant energy conservation

Ramasamy, M. and Thangavel, S. *International Journal of Electric Power & Energy Systems*, 2013, 49, 296–307.

In this study, a novel photovoltaic (PV) fed dynamic voltage restorer (PV-DVR) is proposed to mitigate deep voltage sags, voltage swells and outages on a low voltage residential distribution system during both daytime and night time. In addition to the voltage regulation, the proposed PV-DVR reduces the energy consumption from the utility grid by disconnecting the utility grid from the load through the semiconductor switches, when the PV system generates excessive or equal power to the required load demand during the day time. However, the reduction of energy consumption is always desirable for the reduction of panel tariff and global warming gasses. Further, the use of low step-up DC–DC converter with fuzzy-based perturb and observe (P&O) maximum power point tracking (MPPT) algorithm eliminates the drawback of conventional PV-based DVR by tracking maximum power point of the PV array. Simulation and experimental results are presented to validate the advantage of the proposed system.

14/01659 Inter-provincial clean development mechanism in China: a case study of the solar PV sector

Jacques, D. A. *et al. Energy Policy*, 2013, 57, 454–461.

Climate change mitigation is fast becoming a priority for China. A successful policy of implementing and expanding sustainable development and the use of renewable energy is therefore vital. As well as long-term and near-term targets for installed capacity of renewable energy, in its twelfth 5-year plan, China has created strict and ambitious carbon intensity targets for each province. This study proposes an inter-provincial clean development mechanism to assist in meeting these targets. This mechanism will create potential co-benefits of assisting in sustainable development in lesser developed provinces, increasing local air quality and supporting the growth of China's renewable energy sector. This paper also highlights the potential that this inter-provincial clean development mechanism has in accelerating the growth of the domestic solar photovoltaics (PV) sector, for which the market in China is still in its infancy.

14/01660 Measurement and simulation of hot spots in solar cells

Solheim, H. J. *et al. Energy Procedia*, 2013, 38, 183–189.

Solar cells can have various shunts with various origins and current–temperature characteristics. A solar cell with a local ohmic shunt can heat up during partial shadow conditions due to reverse current through the shunt. Depending on the resulting hot spot size and reverse current, the local temperature can be so high that it can damage the solar module. Under field conditions, if hot spots are detected, it would be worthwhile to decide on a threshold temperature for which a solar module should be decommissioned. This work describes experiments where four single cell modules were made with thermocouples embedded close to hot spots. The temperature development in such modules has been measured by an infrared camera and simulated by a three-dimensional finite element model. The temperature development of a hot spot was computed as a function of hot spot reverse current, reverse voltage, time, hot spot size, hot spot location and ambient temperature. The temperature development in the module is well described by the model. Temperature trends were shown to be a function of shunt size as well as location relative to the edge of the cell.

14/01661 Modeling of fluid flow and heat transfer in a trough solar collector

You, C. *et al. Applied Thermal Engineering*, 2013, 54, (1), 247–254.

This paper analysed the flow and heat transfer processes in a trough solar collector of the direct steam generation (DSG) system. A flow and heat transfer model of the working fluid in the absorber was established and solved using the finite difference method. Experimental results of liquid water and dry air heating processes validated the model. The experimental results, got under the condition that the vacuum in the tube was destroyed, were used to test the developed model. The calculation results of the model agreed with the experimental data. The dynamic characteristics of the collector outlet parameters under variations of solar radiation intensity were analysed in this paper. The impulse response of the DSG system was complex as a short-time fluctuation of the solar radiation notably affected the water region length, the two-phase region length and the steam region length, which led to large fluctuations in the outlet temperature. Therefore, the outlet temperature of the once-through DSG system was difficult to control. Extra heat was required to maintain the normal operation of the system.

14/01662 NiO nanoparticles deposited on graphene platelets as a cost-effective counter electrode in a dye sensitized solar cell

Bajpai, R. *et al. Carbon*, 2013, 56, 56–63.

NiO nanoparticles were deposited homogeneously over few layered graphene platelets (GPs) by pulsed laser ablation. The material was used as an electrocatalyst for the counter electrode (CE) of a dye-sensitized solar cell. GPs were synthesized by oxidation of graphite powder followed by a thermal exfoliation and reduction process. The CE made from GPs with NiO nanoparticles attached (NiO-GP) yielded 3.06% power conversion efficiency which is comparable to a conventional platinum thin film based CE (3.57%). The fill factor and short circuit current density were 0.61 and 7.53 mA/cm^2, respectively. The NiO-GP CE outperformed CEs produced using both unsupported NiO nanoparticles (2.03%) and pristine GPs (2.46%). Catalytic activities of the CEs were analysed using electrochemical impedance spectroscopy. Charge transfer resistances for the two interfaces GP-electrolyte and NiO-electrolyte of the NiO-GP CE were 0.85 and 1.72 Ωcm^2, respectively. These values were much smaller than that of the bare GP (3.96 Ωcm^2) and NiO nanoparticle (20.85 Ωcm^2) based CEs. Thus the catalytic ability of each component in the NiO-GP mixture is better than those of the individual components, indicating a synergistic effect. The resistance for the Pt-electrolyte interface (0.63 Ωcm^2) was only slightly better than that for NiO-GP.

14/01663 Optical design of an aspherical cylinder-type reflecting solar concentrator

Qin, H. *et al. Energy*, 2013, 57, 751–758.

This paper presents a highly efficient solar concentrating mirror. A part of the aspherical cylinder's inner wall defined by a set of specific coefficients a_2, a_4, a_6, a_8, a_{10}, a_{12}, a_{14}, a_{16} and C is used as reflective surfaces of concentrating mirror. Based on the particular aspherical equation and the optical law of reflection, the relationship between the direction vectors of the sunlight beams reflected from the cylindrical inner wall and the coefficients of an aspherical equation, a_2, a_4, a_6, a_8, a_{10}, a_{12}, a_{14}, a_{16} and C has been derived. By optimizing these coefficients, the sunbeams incident on the aspherical cylinder's inner wall can be focused on a very narrow line segment parallel to the cylindrical busbar and form a linear focus (focal line). The particular set of coefficients associated with the particular aspherical equation is obtained by using particle swarm optimization algorithm. The focusing effect of the solar concentrating mirror with respect to the particular set of coefficients is demonstrated by using computer simulations and the experiment. The theoretical results show that this solar concentrat-

ing mirror has a light compression ratio of about 285 to 1. The linear spot can be used as a strong light source or a high temperature heat source.

14/01664 Optimizing performance parameters of graphene–silicon and thin transparent graphite–silicon heterojunction solar cells

An, X. *et al. Carbon*, 2013, 57, 329–337.

The authors investigated heterojunctions of Si with large-area high-quality monolayer and multi-layer graphene, as well as thin transparent graphite. They show that by controlling the transmittance and sheet resistance of large-area graphitic electrodes, it is possible to obtain solar cells with power conversion efficiency (PCE) exceeding 3% without any doping requirements. The calculations indicate that such junctions can form extremely robust interfaces with near-100% internal quantum efficiency. Under optimized doping conditions, power conversion efficiencies increase almost universally by a factor of 2.5. Optimized conditions for reproducibly obtaining cells with PCE > 5% are presented, with the best PCE obtained ~7.5% with short-circuit current density exceeding 24 mA/cm^2.

14/01665 Performance evaluation of directly photovoltaic powered DC PM (direct current permanent magnet) motor – propeller thrust system

Atlam, O. and Kolhe, M. *Energy*, 2013, 57, 692–698.

The photovoltaic (PV)-powered directly coupled electromechanical system has wide applications (e.g. PV-powered cooling fans in greenhouses, PV water pumping systems and solar vehicles). The objective of this work is to analyse the operation of directly PV-powered direct current permanent magnet (DC PM) motor–propeller system for selection of motor parameters. The performance of such a system mainly depends on the incident solar radiation, operating cell temperature, DC motor and propeller load parameters. It is observed that the operating points of the PV DC PM motor–propeller system matches very closely with the maximum power points of the PV array, if the DC PM motor–propeller parameters have been properly selected. It is found that for a specific application of such type of system, matching of torque–speed operating points with respect to the maximum power points of PV array are very important. It is ascertained through results that the DC PM motor's armature resistance, magnetic field constant, starting current to overcome the starting torque and torque coefficient are the main parameters. In designing a PV-powered DC PM motor for a specific application, selection of these parameters are important for maximum utilization of the PV array output. The results of this system are useful for designing of directly PV powered DC PM motor's for aerodynamic applications.

14/01666 Theoretical study on thermal stability of molten salt for solar thermal power

Wei, X. *et al. Applied Thermal Engineering*, 2013, 54, (1), 140–144.

Molten salt (HTS) composed of 53% KNO_3, 40% $NaNO_2$ and 7 wt% $NaNO_3$ has been used as heat transfer media and thermal storage fluid in the solar thermal power, but thermal decomposition will occur at higher temperature because of the oxidation of nitrite to nitrate in the air. In this paper, the reaction mechanism of NO_2^- oxidation is researched by quantum mechanical method. The results show that two components of the transition state ($O_2NO_2^-$) and intermediate ([NO_4^-]) are found in the reaction. This reaction is an exothermic reaction and the activation barrier is 94.0 kJ mol^{-1}. The energy difference of this reaction is very large, so the reaction rate is very slow.

Wind energy

14/01667 A tale of three counties: understanding wind development in the rural Midwestern United States

Mulvaney, K. K. *et al. Energy Policy*, 2013, 56, 322–330.

Understanding the context in which local wind farm development has been accepted by the local community is important for meeting the USA's wind energy goals. To further this understanding in the rural Midwest, the authors investigated three counties in Indiana with varying levels of wind farm development using a mail survey, stakeholder interviews and a review of local newspaper articles and government documents. They found high levels of acceptance for wind energy in general and for local wind farms in all three counties despite the differences in actual development. Multiple statistical methods were employed to identify factors leading to support of wind turbines within the community, but support was so high that no individual factors were identified as statistically significant. The survey and interviews showed that reasons for support of wind energy include economic benefits to the local community, environmental benefits and the protection of the agricultural lifestyle and landscape. Reasons for opposition include concerns about setback distances, impacts on rural lifestyles, and impacts on other types of development. Despite overall community support, the support of the local county governments varied and appears to have greatly impacted wind farm development within their jurisdictions.

14/01668 An integrated control approach for standalone operation of a hybridised wind turbine generating system with maximum power extraction capability

Mendis, N. and Muttaqi, K. *International Journal of Electric Power & Energy Systems*, 2013, 49, 339–348.

This paper presents a novel configuration of a hybrid wind generating system which can be used as a remote area power supply (RAPS) system. The proposed wind energy conversion system consists of a doubly-fed induction generator (DFIG) and a permanent magnet synchronous generator (PMSG) where the latter is connected to the DC bus of the DFIG generator. In addition, a battery storage system is also incorporated into the DC bus to address the demand-generation mismatch. Control strategies for individual system components of the RAPS system are designed with a view to achieve an acceptable level of voltage and frequency regulation while extracting the maximum power from wind. The performance of the proposed RAPS system is investigated in terms of voltage and frequency regulation capability under changing wind and variable load conditions.

14/01669 Approaching wind power forecast deviations with internal ex-ante self-balancing

Scharff, R. *et al. Energy*, 2013, 57, 106–115.

Short-term variations in wind power generation make real-time balancing of load and generation a more challenging task for the transmission system operator (TSO). One issue of interest that could facilitate the efficient integration of wind power is to shift larger parts of the balancing responsibility from the TSO to the power generating companies. The idea is to reduce the real-time balancing need for the TSO by demanding power generating companies to minimize their expected imbalances. To comply with this, power generating companies can re-schedule their production based on updated production forecasts. As a key of the contribution, this paper analyses internal *ex ante* self-balancing, where this re-scheduling is done shortly before the period of delivery and internally within each power generating company. To quantify the value of such a more distributed balancing responsibility, a model has been developed which consists of a sequence of optimization models. Then, possible trading decisions of power generating companies are evaluated in different situations. This is based on a hydro-thermal generation portfolio within the framework of the Nordic electricity market.

14/01670 Determination of cost–potential-curves for wind energy in the German federal state of Baden-Württemberg

McKenna, R. *et al. Energy Policy*, 2013, 57, 194–203.

The new federal government in the German federal state of Baden-Württemberg has set a target for 10% of gross electricity generation from wind energy by 2020. Given that currently around 0.1% of the electricity generation comes from wind energy, this paper examines the technical feasibility and economic costs associated with realizing this goal. The technical potential for wind energy in Baden-Württemberg is determined, along with the costs of electricity generation, which together lead to the derivation of cost–potential-curves. The technical potential is calculated by identifying the available area with the aid of a geographical information system and land use information. With the help of a regional wind atlas, turbine power curves and an assumed wind speed frequency distribution, the spatially distributed electricity generation potential on a district level is estimated. The costs of wind energy are investigated for the year 2010 and projected for the years 2020 and 2030 on the basis of learning curves. The result is a suitable area for wind energy of 2119 km^2, which amounts to 5.9% of the total area of Baden-Württemberg. Depending on the wind turbine selected, a capacity of 18.5 GW up to 24.5 GW could be installed and depending on the hub height and the turbine, an electricity yield of 29.3 TWh up to 40.7 TWh could be generated. The costs of electricity, depending on the type of turbine and the average wind speed, but lie for 2010 between 3.99 and 21.42 €-cents/kWh, reducing by 2030 to 3.33–17.84 €-cents/kWh.

14/01671 Impacts of solidity and hybrid system in small wind turbines performance

Mohamed, M. H. *Energy*, 2013, 57, 495–504.

Wind energy represents a very important source of energy for many countries. Wind energy provides an efficient and an effective solution to reduce fusel fuel consumption as well as pollutant emissions. Vertical axis wind turbines (VAWTs) were originally considered as very promising, before being subrogated by the present, horizontal axis turbines. There is now a resurgence of interests for VAWTs, in particular Darrieus turbines. VAWTs like the Darrieus turbine appear to be particularly promising for the conditions of low wind speed, but

suffer from a low efficiency compared to horizontal axis turbines. Additionally, VAWTs are not always self-starting, which is a major drawback. The present paper introduces the main problem of the self-starting capability of Darrieus turbine and investigates some techniques to improve this drawback. The effect of the turbine solidity and the usage of hybrid system between drag and lift types have been investigated in this paper numerically using a computational fluid dynamics technique and experimentally. A considerable improvement of the H-rotor Darrieus turbine self-starting capability can be obtained by these techniques.

14/01672 Incorporating load variation and variable wind generation in service restoration plans for distribution systems

Zidan, A. and El-Saadany, E. F. *Energy*, 2013, 57, 682–691.

A service restoration process is achieved through the switching actions of the sectionalizing and tie switches in distribution feeders. After the faults have been located and isolated, restoration plans are applied in order to minimize the de-energized consumer load and the number of switching operations. All of these objectives are converted to monetary costs, which are then added together into a global objective. The solution to the problem, which is based on a genetic algorithm, is then aimed at achieving the minimum cost. In this work, numerous practical aspects related to service restoration have been considered, such as variations in the load and the priorities of the customers, price discounts for in-service customers based on their participation in a load-curtailment scheme that permits other customers to be supplied, the presence of manual and automated switches, and the incorporation of distributed generation (dispatchable and wind-based distributed generation units) in the restoration process. The constraints involved include voltage limits, line current limits and radial topology.

14/01673 Irregular-shape wind farm micro-siting optimization

Gu, H. and Wang, J. *Energy*, 2013, 57, 535–544.

Landscape constraints inevitably cause the irregularity of the shape or boundary of a wind farm, which was not fully considered in previous literature. In this paper, a single-boundary constraint model and a novel multi-boundary constraint model incorporated with ray intersection method are developed to quantify the irregular boundary constraint for wind farm micro-siting optimization. In order to obtain high-fidelity wind farm shape information, an edge detection algorithm is employed to extract wind farm contour data from digital maps, and an optimal polygonal approximation algorithm is applied to compress the contour data so as to make the computation of boundary constraints less time-consuming. Simulations of four commercial wind farms comprehensively demonstrate the effectiveness of the proposed boundary constraint models and the significance of irregular-shape wind farm micro-siting optimization.

14/01674 Multibody dynamics of floating wind turbines with large-amplitude motion

Wang, L. and Sweetman, B. *Applied Ocean Research*, 2013, 43, 1–10.

A new approach to multibody dynamics is investigated by treating floating wind turbines as multibody systems. The system is considered as three rigid bodies: the tower, nacelle and rotor. Three large-amplitude rotational degrees of freedom (DOFs) of the tower are described by 1–2–3 sequence Euler angles. Translation of the entire system is described by Newton's second law applied to the centre of mass (CM) of the system and transferred to three translational DOFs of the tower. Additionally, two prescribed DOFs governed by mechanical control, nacelle yaw and rotor spin, are combined with the six DOFs of the tower to formulate the eight-DOF equations of motion (EOMs) of the system. The CM of the system is generally time varying and not constrained to any rigid body due to the arbitrary location of the CM of each body and relative mechanical motions among the bodies. The location of the CM being independent of any body is considered in both the solution to three translational DOFs and the calculation of angular momentum of each body for three rotational DOFs. The theorem of conservation of momentum is applied to the entire multibody system directly to solve six unknown DOFs. Motions computed using the six non-linear EOMs are transformed to each body in a global coordinate system at every time-step for use in the computation of hydrodynamics, aerodynamics and restoring forcing, which preserves the non-linearity between external excitation and structural dynamics. The new method is demonstrated by simulation of the motion of a highly compliant floating wind turbine. Results are verified by critical comparison with those of the popular wind turbine dynamics software FAST.

14/01675 Offshore wind energy policy for India – key factors to be considered

Mani, S. and Dhingra, T. *Energy Policy*, 2013, 56, 672–683.

India's economy has grown at a healthy pace over the past few years. To sustain this growth, the power sector needs to build additional generation capacity. However, continued dependence on fossil fuels for electricity generation capacity is not sustainable. Renewable energy resources forms a small portion (25 GW, ~12%) of India's overall power generation today (202 GW). The share of wind energy (17 GW) is 67% of the total renewable energy production. The contribution from offshore wind farms is non-existent, as all the wind energy generated in India is only through onshore wind farms. India needs a policy framework to encourage the development of offshore wind farms. Several European countries have effective offshore wind energy policies that have helped them to accelerate the growth of their offshore wind energy sector. This paper does an exhaustive literature survey to identify 21 building blocks of a successful offshore wind energy policy initiative adopted by select European countries. These have been classified under five broad categories: government support, fiscal and quota-based incentives, availability of local expertise, capital for investments and building an enabling ecosystem. These categories can be used by India in order to develop its own offshore wind energy policy.

14/01676 Optimal offering strategy considering the risk management for wind power producers in electricity market

Hosseini-Firouz, M. *International Journal of Electric Power & Energy Systems*, 2013, 49, 359–368.

This paper provides a technique based on stochastic programming to optimally solve the wind power problem faced by the uncertainty. Uncertainties regarding the wind availability, market prices, and balancing energy needs are considered throughout the paper. The objective of this paper is to derive the best offering strategy for a wind power producer in a short-term electricity market, while limiting the risk of expected profit and required reserve due to wind speed forecast volatility. Risk aversion is explicitly modelled using the conditional value-at-risk methodology. ARIMA techniques are used to predict next-day electricity prices and wind speed forecast. For more performance the probability distribution function of the error between forecasted value and realized value to scenario generation is used. A realistic of numerical case studies demonstrates the interest and the effectiveness.

14/01677 Political and institutional analysis of the successes and failures of China's wind power policy

Zhang, S. *et al. Energy Policy*, 2013, 56, 331–340.

This paper identifies and explains how political and institutional factors have determined the relative successes and failures of China's wind power policy over the period 2005–2011. It finds that China has made significant progress in pursuing its wind power policy in terms of cumulative installed capacity, wind turbine manufacturing industry development and wind turbine cost, and argues that these achievements can be attributed to the political motives and institutional arrangements of the Chinese government as well as to institutional changes. On the other hand, the paper finds that there are two prominent policy failures, namely the low proportion of grid-connected capacity and the rising trend of wind turbine incidents. These have undermined the efficiency and effectiveness of China's wind power program. The paper holds that the institutional sources for the first policy failure lies in the preference for setting wind power development targets in terms of installed capacity rather than generation and in co-ordination problems while the second policy failure lies in the lack of state technical codes for wind power integration and the unfair competition from the large state-owned power companies. The paper contributes to the academic literature on the political and institutional roles in China's wind power policy.

14/01678 States of transmission: moving towards large-scale wind power

Fischlein, M. *et al. Energy Policy*, 2013, 56, 101–113.

Efforts to plan and site transmission for wind power cannot currently keep pace with wind power development. The very nature of wind power, whether distributed or intermittent, challenges traditional models of electricity grid development. Much of the decision authority for transmission is located at the state level, creating tensions between a system-wide need for transmission capacity and the local nature of planning and implementation. This study identifies and discusses barriers for wind power transmission and highlights the critical role of states and state policies in expanding and transforming the electricity grid to accommodate large-scale wind power. Drawing on extensive interview data with energy stakeholders, this study presents a comparative case study of state-level contexts linking wind and transmission in Montana, Minnesota, and Texas. Stakeholders were found to portray transmission challenges and solutions for wind power based on the character of the local transmission grid, their status as power importer, exporter or self-sufficient state, and the role wind already plays in the power supply.

Others, including economics

14/01679 An in-depth assessment of hybrid solar–geothermal power generation
Zhou, C. *et al. Energy Conversion and Management*, 2013, 74, 88–101.
A major problem faced by many standalone geothermal power plants, particularly in hot and arid climates such as Australia, is the adverse effects of diurnal temperature change on the operation of air-cooled condensers which typically leads to fluctuation in the power output and degradation of thermal efficiency. This study is concerned with the assessment of hybrid solar–geothermal power plants as a means of boosting the power output and where possible moderating the impact of diurnal temperature change. The ultimate goal is to explore the potential benefits from the synergies between the solar and geothermal energy sources. For this purpose the performances of the hybrid systems in terms of power output and the cost of electricity were compared with that of stand-alone solar and geothermal plants. Moreover, the influence of various controlling parameters including the ambient temperature, solar irradiance, geographical location, resource quality, and the operating mode of the power cycle on the performance of the hybrid system were investigated under steady-state conditions. Unsteady-state case studies were also performed to examine the dynamic behaviour of hybrid systems. These case studies were carried out for three different Australian geographic locations using raw hourly meteorological data of a typical year. The process simulation package Aspen-HYSYS was used to simulate plant configurations of interest. Thermodynamic analyses carried out for a reservoir temperature of 120 °C and a fixed brine flow rate of 50 kg/s revealed that under Australian climatic conditions (with a typical ambient temperature of 31 °C in summer) a hybrid plant would outperform stand-alone geothermal and solar power plants if at least 68% of its energy input is met by solar energy (i.e. a solar energy fraction of ≈68%). This figure drops to about 19% for reservoir temperatures greater than 170 °C. Case studies also showed that, for a mid-range reservoir temperature of 150 °C, the cost of electricity production can be reduced by 20% when a hybrid plant is used instead of the stand-alone enhanced geothermal system.

14/01680 Beyond commonplace biofuels: social aspects of ethanol
Ribeiro, B. E. *Energy Policy*, 2013, 57, 355–362.
Biofuels policies and projects may lead to environmental, economic and social impacts. A number of studies point out the need to deliver comprehensive sustainability assessments regarding biofuels, with some presenting analytical frameworks that claim to be exhaustive. However, what is often found in the literature is an overexploitation of environmental and economic concerns, by contrast to a limited appraisal of the social aspects of biofuels. Building on a systematic review of the peer-reviewed literature, this paper discusses the social constraints and strengths of ethanol, with regard to the product's lifecycle stages and the actors involved. Its objective is to contribute to the development of social frameworks to be used in assessing the impact of ethanol. Main findings indicate that ethanol developments can increase the levels of social vulnerability, although there is little evidence in the literature regarding the positive and negative social impacts of first-generation ethanol and potential impacts of cellulosic ethanol. Further work is needed on the formulation of social criteria and indicators for a comprehensive sustainability assessment of this biofuel. Policy makers need to internalize the social dimension of ethanol in decision-making to prevent public opposition and irreversible social costs in the future.

14/01681 Economic factors influencing potential use of cellulosic crop residues for electricity generation
Maung, T. A. and McCarl, B. A. *Energy*, 2013, 56, 81–91.
This study examines cellulosic crop residues for biopower production in the context of greenhouse gas (GHG) emissions mitigation. The authors use sector modelling to simulate future market potential for biopower production from crop residues. The findings suggest that in order for crop residues to have any role in electricity generation either the carbon or CO_2 equivalent GHG price must rise to about $15 per ton or the price of coal has to increase to about $43 per ton. Crop residues with higher heat content were found to have greater opportunities in biopower production than the residues with lower heat content. In addition, the evidence shows that improvements in crop yields do not have much impact on biopower production. However, the energy recovery efficiency does have significant positive impact but only if the CO_2 equivalent price rises substantially. Moreover, this analysis indicates the desirability of cofiring biomass as opposed to 100% replacement because this reduces transportation cost and increases the efficiency of heat recovery. In terms of policy implications, imposing carbon emission pricing could be an important step in inducing electric power producers to include biomass feedstocks in their fuel-mix power generation portfolios and achieve GHG emission reductions.

14/01682 Flap gate farm: from Venice lagoon defense to resonating wave energy production. Part 1: natural modes
Sammarco, P. *et al. Applied Ocean Research*, 2013, 43, 206–213.
This study considers a flap-gate farm, i.e. a series of P arrays, each made by Q neighbouring flap gates, in an infinitely long channel. The authors show that there are $P \times (Q-1)$ natural modes and determine their eigenfrequencies and modal forms. When the distance between the arrays goes to infinity the eigenfrequencies converge to the $Q-1$ values given by Li and Mei in an earlier study. For an *ad hoc* combination of channel geometry and flap gate characteristics, modal excitation can give significantly larger response than for the case of a single or a sparse gate system. This aspect is relevant for the design of an optimal gate farm wave energy converter.

14/01683 Renewable energy sector development in the Caribbean: current trends and lessons from history
Shirley, R. and Kammen, D. *Energy Policy*, 2013, 57, 244–252.
Island regions and isolated communities represent an understudied area of not only clean energy development but also of innovation. Caribbean states have for some time shown interest in developing a regional sustainable energy policy and in implementing measures which could help to protect its member states from volatile oil markets while promoting reliance on local resources. Here four case studies of renewable energy advancements being made by public utility companies and independent energy companies in the Caribbean are examined. The authors attempt to locate renewable energy advances in a broader historical framework of energy sector development, indicating a few policy lessons. It was found that that different degrees of regulatory and legislative sophistication have evolved in different islands. Islands should have specialized policy focus, contrasting the *ad hoc* nature of current regional energy policy discussion. The authors also conducted a cost-benefit analysis which shows that these early, innovative alternative energy projects show themselves to be both profitable and significant sources of emissions reduction and job creation. This lends support to the potential benefits of regional energy policy.

14/01684 The feasibility of synthetic fuels in renewable energy systems
Ridjan, I. *et al. Energy*, 2013, 57, 76–84.
While all other sectors had significant renewable energy penetrations, transport is still heavily dependent on oil displaying rapid growth in the last decades. There is no easy renewable solution to meet transport sector demand due to the wide variety of modes and needs in the sector. Nowadays, biofuels along with electricity are proposed as one of the main options for replacing fossil fuels in the transport sector. The main reasons for avoiding the direct usage of biomass, i.e. producing biomass derived fuels, are land use shortages, limited biomass availability, interference with food supplies, and other impacts on the environment and biosphere. Hence, it is essential to make a detailed analysis of this sector in order to match the demand and to meet the criteria of a 100% renewable energy system in 2050. The purpose of this paper is to identify potential pathways for producing synthetic fuels, with a specific focus on solid oxide electrolyser cells combined with the recycling of CO_2.

14 FUEL SCIENCE AND TECHNOLOGY

Fundamental science, analysis, instrumentation

14/01685 A comparison of innovation policy in the smart grid industry across the pacific: China and the USA
Lin, C.-C. *et al. Energy Policy*, 2013, 57, 119–132.
Utilities are increasing their investment in smart grid technologies because of the rising demand for electricity, the aging transmission and distribution infrastructure in developed countries and the need for real-time visibility of energy supply and demand to optimize service reliability and cost. Government policies are contributing to this rising investment in the smart grid in many countries around the globe. Using

Rothwell and Zegveld's innovation policy framework as a starting point, this paper compares innovation policy in smart grids across the Pacific; specifically, China and the USA. This research describes the policy tools used by both countries and presents results that indicate national preferences for innovation policy that differ in the ways in which they are linked with the state of the power system. China has preferred to use 'supply-side policy,' which focuses on 'public enterprise, scientific and technical development and legal regulation'. The USA has preferred to use 'environmental-side policy', which focuses on 'scientific and technical development, financial, political and public enterprise.' This paper also describes in detail a number of innovation policies being pursued in the smart grid industry in both China and the USA.

14/01686 A highly accurate technique for the solution of the non-linear point kinetics equations

Picca, P. *et al. Annals of Nuclear Energy*, 2013, 58, 43–53.

A novel methodology for the solution of non-linear point kinetic (PK) equations is proposed. The technique, based on a piecewise constant approximation, is enhanced by explicitly accounting for the feedback and the reactivity variation within a time step through an iterative cycle. High accuracy is achieved by introducing a sub-mesh for the numerical evaluation of integrals involved and by correcting the source term to include the non-linear effect on a finer time scale. The resulting enhanced piecewise constant approximation (EPCA) is tested on a set of classical linear problems with several types of reactivity insertions (step, linear, sinusoidal, zig-zag) and shows extreme accuracy (to nine digits) even when large time steps are considered (i.e. 100 times the neutron mean life). Non-linear reactor kinetics is then considered and compared to highly accurate results obtained via convergence acceleration. Its accuracy and the fast convergence make the EPCA algorithm particularly attractive for applications.

14/01687 A new correlation for estimating thermal conductivity of pure ionic liquids

Shojaee, S. A. *et al. Fluid Phase Equilibria*, 2013, 354, 199–206.

In the present study, a new correlation with both correlative and extrapolative capabilities is proposed for thermal conductivity of the pure ionic liquids (ILs) and the optimum values of its fitting parameters were obtained by a genetic algorithm. All of all, 209 data points of 21 ILs were collected from previously published literature. The collected data were divided into two different subsets namely training (143 data points) and testing (66 data points) subsets. Training subset was used to find the optimum values of the fitting parameters of the proposed correlation. After that, the extrapolative and correlative capabilities of the proposed correlation was tested by testing data subset was not utilized during the training stage. The average absolute relative deviation percent (AARD %) during the training stage was 5.22%, while the results revealed AARD % of 10.76% for testing stage. In general, the overall results revealed a rather good accuracy of the proposed correlation especially considering its extrapolative capability. Finally, the obtained results by the proposed correlation were compared with those obtained by different available correlations including group contribution and artificial neural network approach which shows a good functionality of the proposed correlation.

14/01688 A new hybrid bacterial foraging and simplified swarm optimization algorithm for practical optimal dynamic load dispatch

Azizipanah-Abarghooee, R. *International Journal of Electric Power & Energy Systems*, 2013, 49, 414–429.

This paper presents a novel approach to depict the practical constraints of generator units such as reserve constraints, prohibited operating zones and valve-point effects in the optimal dynamic dispatch problem. Determining the power generation output of units at minimum total fuel cost a dynamic environment with ramp rate limits to satisfy load demand and transmission losses is too complicated and has a lot of local optima in its search space. In addition, the proposed problem has a non-linear, non-convex, non-smooth, multi-modal, non-separable, and non-differentiable nature. In order to overcome above problems a new hybrid technique, based on bacterial foraging and simplified swarm optimization algorithms combined with a new mutation operator and opposition-based initialization is proposed to restraint the premature convergence of the solutions. Therefore, the bacteria in chemo-tactic procedure are moved in short or long steps as well as swimming movements. Furthermore, to increase the diversity of the solution of the search space a novel self-adaptive mutation strategy which profits from four mutation rules is implemented. For more validation the simulation results are applied on four small-, medium- and large-scale systems with 5, 10, 30 and 100 units and compared with those of other methods in the area.

14/01689 A novel model for risk assessment of adjacent buildings in tunneling environments

Zhang, L. *et al. Building and Environment*, 2013, 65, 185–194.

This paper presents a novel model to assess the risk of adjacent buildings in tunnelling environments based on extended cloud model (ECM). ECM is an organic integration of extension theory (ET) and cloud model (CM), where ET is appropriately employed to flexibly expand the variable range from [0, 1] to $(-\infty, +\infty)$, and CM is used to overcome the uncertainty of fuzziness and randomness during the gradation of evaluation factors. An integrated interval recognition approach to determine the boundary of risk related intervals is presented, with both actual practices and group decisions fully considered. The risk level of a specific adjacent building is assessed by the correlation to the cloud model of each risk level. A confidence indicator θ is proposed to illustrate the rationality and reliability of evaluating results. Ten buildings adjacent to Wuhan Metro Line Two are randomly chosen among hundreds of adjacent buildings for a case study, and the results have proved to be consistent with the actual situation. Compared with other traditional evaluation methods, ECM has been verified to be a more competitive solution with no demands on training data. The original data can be directly entered into ECM without a normalization procedure, avoiding the potential information loss. ECM can be offered as a decision support tool for the risk assessment in urban tunnelling construction and worth popularizing in other similar projects.

14/01690 Ambient-pressure photoelectron spectroscopy for heterogeneous catalysis and electrochemistry

Kaya, S. *et al. Catalysis Today*, 2013, 205, 101–105.

The authors describe the design and capabilities of a new ambient-pressure X-ray photoelectron spectroscopy system at the Stanford Synchrotron Radiation Lightsource. A unique feature of this system is that samples are illuminated at grazing incidence and with a tightly focused beam, which allows a 50 μm aperture to be placed in the first differential pumping stage of the lens system of the electron spectrometer. The low conductance of the aperture enables surface-sensitive electron spectroscopy of solid surfaces, liquids, and solid–liquid interfaces to be performed *operando* at pressures as high as 100 Torr. The instrument can also be used to obtain polarization-resolved X-ray absorption spectra using Auger-electron-yield detection. Results for Pt surfaces in ambient-pressure gas environments and for liquid water are presented.

14/01691 An efficient shock capturing algorithm to the extended Boussinesq wave equations

Fang, K. *et al. Applied Ocean Research*, 2013, 43, 11–20.

A hybrid finite-volume and finite-difference method is proposed for numerically solving the two-dimensional extended Boussinesq equations. The governing equations are written in such a way that the convective flux is approximated using finite volume method while the remaining terms are discretized using finite difference method. Multi-stage (MUSTA) scheme, instead of commonly used HLL or Roe schemes, is adopted to evaluate the convective flux as it has the simplicity of centred scheme and accuracy of upwind scheme. The third-order Runge–Kutta method is used for time marching. Wave breaking and wet–dry interface are also treated in the model. In addition to model validation, the emphasis is given to compare the merits and limitations of using MUSTA scheme and HLL scheme in the model. The analytical and experimental data available in the literature have been used for the assessment. Numerical tests demonstrate that the developed model has the advantages of stability preserving, shock-capturing and numerical efficiency when applied in the complex near-shore region. Compared with that using HLL scheme, the proposed model has comparable numerical accuracy, but requires slightly less computation time and is much simpler to code.

14/01692 Behaviour of spreading molten metal drops deposited by fusion

Chapuis, J. *et al. Experimental Thermal and Fluid Science*, 2013, 48, 29–36.

Liquid droplet deposition on solid surfaces has an important role in the industrial and research activities. The behaviour of such deposit is influenced by volume and interfacial phenomena and involves a large number of mechanisms such as gravity effect, mass transfer, capillary forces, and wetting. For the case of metal deposition the analysis of the problem is more complex because of the importance of thermal effects, involving steep gradients and phase changes. A unique experimental approach is presented in order to study the evolution of the spreading of a large drop of liquid metal called 'macro-drop'. The objective of this work is to supply qualitative and quantitative information during the deposit of liquid metal in relation with process parameters. The overall shape of the macro-drop, especially its spreading and contact angles, is studied in detail. The gradual spreading of the macro-drop is mainly governed by mass and heat transfers. The initial rapid spreading is due to kinetic energy of depositing droplets and direct arc heating on the solid target. All experimental results are analysed in the light of process parameters to identify the physical mechanisms involved and appreciate their effects on the behaviour of such a macro-drop.

14/01693 Bubble shape under the action of electric forces

Di Marco, P. *et al. Experimental Thermal and Fluid Science*, 2013, 49, 160–168.

This study of bubble dynamics in adiabatic conditions (i.e. with no heat and mass transfer) considers the fundamental physics ruling the evolution of the interface, and opens the way to the comprehension of more complex heat and mass transfer issues involving them. An external electric field is applied to the system to investigate the potentiality of this technique to enhance phase separation and heat transfer. A new numerical method for electrohydrodynamic action on a growing bubble has been developed combining the volume of fluid and level-set methods. To experimentally validate it, well-defined and simple boundary conditions have been selected: all the forms of heat and mass transfer have been excluded from the system, and an axisymmetric electric field configuration has been chosen in order to adopt a two-dimensional simulation. In the experimental apparatus, a steady bubble stemming from an orifice in a still fluid (FC-72) has been produced, and a dc potential up to 20 kV was applied to a ring-shaped electrode coaxial with the orifice. In this way, in a first instance, all the dynamical effects have been eliminated, and a clear location of the three-phase contact line, which is pinned to the orifice, has been defined. The bubble profile obtained from the experiment has been digitized and compared successfully with the outcomes of the numerical method. Furthermore, the study of the local curvature of the interface allowed the development of a new theory of the local electrical stress to be included in the capillary equation, which compares well with experimental data. Finally, the validated numerical method has been used to predict the bubble shape in the absence of gravity, in preparation of microgravity experiments.

14/01694 Calibrating a combined energy systems analysis and controller design method with empirical data

Murphy, G. B. *et al. Energy*, 2013, 57, 484–494.

The drive towards low carbon constructions has seen buildings increasingly use many different energy systems simultaneously to control the human comfort of the indoor environment; such as ventilation with heat recovery, various heating solutions and applications of renewable energy. This paper describes a dynamic modelling and simulation method (Inverse Dynamics-based Energy Assessment and Simulation, IDEAS) for analysing the energy use of a building and its complex servicing systems. The IDEAS case study presented in this paper is based on small perturbation theory and can be used for the analysis of the performance of complex energy systems and also for the design of smart control systems. This paper presents a process of how any dynamic model can be calibrated against a more empirical based data model, in this case the UK government's standard assessment procedure. The research targets of this work are building simulation experts for analysing the energy use of a building and also control engineers to assist in the design of smart control systems for dwellings. The calibration process presented is transferable and has applications for simulation experts to assist in calibrating any dynamic building simulation method with an empirical based method.

14/01695 Changing the regulation for regulating the change: innovation-driven regulatory developments for smart grids, smart metering and e-mobility in Italy

Lo Schiavo, L. *et al. Energy Policy*, 2013, 57, 506–517.

For a long time considered as technologically mature, electric systems are now facing a period of rapid evolution, inspired by climate change concerns. Several studies show that current regulation of natural monopolies does not offer sufficient incentives for network operators (and network users) to participate in this process. Taking Italy as a case study, this paper analyses how energy regulation can change to support the current transformation. The authors describe the recent regulatory interventions in the domain of smart grids, smart metering and electromobility, with a specific emphasis on the provisions aimed at fostering innovation – an issue that until recently has received almost no attention in the literature nor in the practice of regulation. The progress observed in the course of this study is considerable in all new areas of concern, and, above all, in the regulator's commitment to provide the right incentives for investments in demonstration projects: the acquisition of experience is regarded as essential to move to more sophisticated regulatory instruments. Finally, regulation is also increasingly concerned with network users, both traditional and new, with the objective to stimulate more active behaviours.

14/01696 Coupled SPHS–BEM method for transient fluid–structure interaction and applications in underwater impacts

Zhang, A. M. *et al. Applied Ocean Research*, 2013, 43, 223–233.

The coupled smoothed particle hydrodynamics (SPH) shell (SPHS)–boundary element method (BEM) method is proposed for transient fluid–structure interaction problems: SPHS BEM is selected to discretize shell structures, the second-order doubly asymptotic approximations (DAA_2) of the BEM is chosen to analyse the flow-field. BEM can remedy the expensive costs for three-dimensional SPH, yet SPHS provides a structural solver for BEM. The coupled method is attractive, since only a layer of SPHS particles and a piece of flow-field boundary elements are needed to be modelled; the compatibility conditions of the coupled surface are performed with moving least square function. The final two benchmarks on underwater impacts prove the feasibility, stability and accuracy of the proposed method.

14/01697 Development of a control algorithm employing data generated by a white box mathematical model

Maia, A. A. T. *et al. Applied Thermal Engineering*, 2013, 54, (1), 120–130.

The optimization of vapour compression refrigeration systems to improve their energetic efficiency has become an important goal of the field of thermal engineering. To this end, a refrigeration capacity control that operates through the continuous adjustment of the compressor speed and the opening of the expansion valve has been utilized. To develop the algorithm responsible for these adjustments, it is necessary to gather information about the refrigeration system's dynamics. This information is generally obtained from experimental data, which is not always available. This study presents the development of a concentric tube evaporator mathematical model. After being validated with experimental data, this mathematical model was utilized to generate the information on the system dynamics that is necessary to project an adaptive multivariable controller. The obtained results showed that the proposed model can be used to describe refrigeration machine dynamics and that this information can be used in the controller design.

14/01698 Evaluation of inhibitory effect of TiO_2 nanocoatings against microalgal growth on clay brick façades under weak UV exposure conditions

Graziani, L. *et al. Building and Environment*, 2013, 64, 38–45.

Microalgal growth largely affects the aesthetical properties of building façades worldwide. It causes biodeterioration of building materials and, in a later stage, it can compromise integrity of the elements and their durability. Recently, the use of nanotechnology to prevent the growth of microalgae is rising. One of the most widespread and promising material is titanium dioxide (TiO_2). Photocatalytic properties of TiO_2 inhibit biofouling of microalgae when this coating is stimulated by UV radiation coming from the sun or from artificial light. In this study, the biocide effect of TiO_2 coatings applied on clay brick specimens under weak UV radiation was assessed. Results revealed that TiO_2 nanocoating was not able to fully prevent microalgal biofouling, but under optimal UV exposure conditions for the growth of microalgae it efficaciously prevented the adhesion of these microorganisms on the treated substrates through the formation of a superficial water film. This property resulted in a good self-cleaning efficiency of TiO_2.

14/01699 Excitation functions of (*n*,2*n*) reactions for stable lead isotopes from reaction threshold to 20 MeV

Jeremiah, J. J. *et al. Annals of Nuclear Energy*, 2013, 56, 44–47.

The excitation functions for (*n*,2*n*) reactions from reaction threshold to 20 MeV on four stable lead isotopes ^{204}Pb, ^{206}Pb, ^{207}Pb and ^{208}Pb were calculated using Talys-1.2 nuclear model code, this essentially involves fitting a set of global parameters. An excellent agreement between the calculated and experimental data is obtained. The level densities and effective imaginary potential were studied to obtain the best fit of the excitation functions. The cross sections were calculated by invoking suitable options for global optical model potential, microscopic level densities from Goriely's table, Hauser–Feshbach model for equilibrium calculations, the two-component exciton model by Kalbach for pre-equilibrium calculations in the Talys input file. The results of the present study reveal that the theoretical estimation of the cross-sections match fairly well with the experimental data (EXFOR database) as well as with the evaluated data files (ENDF/VII.0, JENDL-4.0, CENDL-3.1). This is of importance to the validation of nuclear model approaches with increased predictive power.

14/01700 Experimental investigation on friction factor in pipes with large roughness

Huang, K. *et al. Experimental Thermal and Fluid Science*, 2013, 50, 147–153.

This paper experimentally and theoretically investigated the differences on friction factor in rough pipes with large surface roughness. Deviation from theoretical theory for laminar flow in rough tubes was confirmed again. The product of fRe was larger than 64 and can be predicted as a quadratic equation of relative roughness. Earlier transition between flow regimes was observed. The critical Reynolds number between flow regimes decreased as the relative roughness increased. The range of Reynolds number for transitional flow regime gradually reduces with an increase in surface roughness. When relative roughness reach peak ($\Delta/d = 1/2.4$), transitional flow regime disappeared. Navier–Stokes equation was used to analyse the differences on flow behaviour. It indicates flow obstruction of surface roughness

caused curve flow for laminar flow in porous medium and linear law for laminar flow in porous media may be an approximate expression by neglecting the inertial forces at low Reynolds number.

14/01701 Experimental measurement of cooling tower emissions using image processing of sensitive papers

Ruiz, J. *et al. Atmospheric Environment*, 2013, 69, 170–181.

Cooling tower emissions are harmful for several reasons such as air pollution, wetting, icing and solid particle deposition, but mainly due to human health hazards (i.e. Legionella). There are several methods for measuring drift drops. This paper is focused on the sensitive paper technique, which is suitable in low drift scenarios and real conditions. The lack of an automatic classification method motivated the development of a digital image process algorithm for the sensitive paper method. This paper presents a detailed description of this method, in which, drop-like elements are identified by means of the Canny edge detector combined with some morphological operations. Afterwards, the application of a J48 decision tree is proposed as one of the most relevant contributions. This classification method allows us to discern between stains whose origin is a drop and stains whose origin is not a drop. The method is applied to a real case and results are presented in terms of drift and PM_{10} emissions. This involves the calculation of the main features of the droplet distribution at the cooling tower exit surface in terms of drop size distribution data, cumulative mass distribution curve and characteristic drop diameters. The log-normal and the Rosin–Rammler distribution functions have been fitted to the experimental data collected in the tests and it can been concluded that the first one is the most suitable for experimental data among the functions tested (whereas the second one is less suitable). Realistic PM_{10} calculations include the measurement of drift emissions and total dissolved solids as well as the size and number of drops. Results are compared to the method proposed by the US Environmental Protection Agency assessing its overestimation. Drift emissions have found to be 0.0517% of the recirculating water, which is over the Spanish standards limit (0.05%).

14/01702 Experimental studies on the anti-uplift behavior of the suction caissons in sand

Gao, Y. *et al. Applied Ocean Research*, 2013, 43, 37–45.

A series of model tests was conducted in sand to explore the anti-uplift behaviour of suction caissons, considering the effects of aspect ratios, load inclination angles and loading positions. This paper emphasizes on analysing the deformation characteristic and the mechanism of the suction caissons under various loading conditions. The movement modes of the suction caisson are different when the load inclination angle increases from 0° to 90° corresponding to various mooring positions. The pull-out bearing capacity decreases with load inclination angles increasing. When the load inclination angle changes from 0° to 60°, the bearing capacity reduces more significantly than that between inclination angle of 60° and 90°. While the load inclination angle is relatively small, the pull-out capacity of the suction caisson decreases after reaching the peak as the loading position moves downwards. Moreover, the optimum loading position locates between two-thirds and three-quarters of the caisson length. The optimum loading position is at the bottom of the caisson when the load inclination angle exceeds 60°. However, the influence of the loading position on the pull-out capacity of the caisson can be ignored while the load inclination angle equals to 90°. The pull-out bearing capacity increases as the aspect ratio increases but the aspect ratio has no effect on the deformation characteristic of the suction caisson.

14/01703 Highly efficient low voltage electron emission from directly spinnable carbon nanotube webs

Hojati-Talemi, P. *et al. Carbon*, 2013, 57, 169–173.

Two methods for increasing the number of free carbon nanotube (CNT) tips in carbon nanotube webs (CNTW) and improving their field emission (FE) performance are proposed. It was observed that by laterally compressing samples by 35% it is possible to improve FE performance to some extent, with further compression leading to a loss of FE properties due to folding of webs and adhesion between CNT tips. Multilayered samples were also studied and it was found that samples with successive layers in which the orientation of the nanofibres in successive layers was the same, increased inter-bundle van der Waals forces, leading to more compact webs with no improvement in FE performance. However, it was found that if the fibres in successive layers were perpendicular to each other the inter-bundle attraction was minimized, maximizing the number of active CNT tips and yielding materials that exhibit the best FE performance reported for any material to date.

14/01704 Hydroelastic interaction between obliquely incident waves and a semi-infinite elastic plate on a two-layer fluid

Lin, Q. and Lu, D. Q. *Applied Ocean Research*, 2013, 43, 71–79.

The hydroelastic response of a semi-infinite thin elastic plate floating on a two-layer fluid of finite depth due to obliquely incident waves is investigated. The upper and lower fluids with different densities separated by a sharp and stable interface are assumed to be inviscid and incompressible and the motion to be irrotational. Simply time-harmonic incident waves of the surface and interfacial wave modes with a given angular frequency are considered within the framework of linear potential flow theory. With the aid of the methods of matched eigenfunction expansion and the inner product of the two-layer fluid, a closed system of simultaneous linear equations is derived for the reflection and transmission coefficients of the series solutions. Based on the dispersion relations for the gravity waves and the flexural–gravity waves in a two-layer fluid and Snell's law for refraction, the authors obtain a critical angle for the incident waves of the surface wave mode and three critical angles for the incident waves of the interfacial wave mode, which are related to the existence of the propagating waves. Graphical representations of the series solutions show the interaction between the water waves and the plate. The effects of several physical parameters, including the density and depth ratios of the fluid and the thickness of the plate, on the wave scattering and the hydroelastic response of the plate are studied. It is found that the variation of the thickness of the plate may change the wave numbers and the critical angles. The density ratio is the main factor to influence the wave numbers of the interfacial wave modes. Finally, the stress state is considered.

14/01705 Ice nucleation activity of bacteria isolated from cloud water

Joly, M. *et al. Atmospheric Environment*, 2013, 70, 392–400.

Some gammaproteobacteria can catalyse ice formation thereby potentially contributing to the induction of precipitation in super-cooled clouds and subsequently to bacterial deposition. Forty-four bacterial strains from cloud water were screened for their capacity to induce freezing. Seven strains (16%) were active at −8 °C or warmer and were identified as *Pseudomonas syringae*, *Xanthomonas* spp. and *Pseudoxanthomonas* sp. Phylogenetic analysis revealed that the *P. syringae* strains in clouds at the Puy de Dôme belonged to clades that are among the most infrequently detected in the environment, while widespread clades were absent suggesting some extent of selection or unusual biogeography of the bacteria at the sampling site. Three strains induced freezing at −3 °C while the others nucleated ice at −4 to −6 °C. The freezing profiles revealed that the peaks of activity were centred around −3.5, −5 and/or −8.5 °C depending on the strain. The frequency of ice-nuclei (IN) per cell at −6 °C was generally below 0.5% and reached up to 4.2% in one strain. It was estimated that clouds influenced by vegetated areas would carry between less than 1 and ∼500 bacterial IN mL^{-1} of water active between −3 and −10 °C depending on the season. These data will contribute to modelling the impact of bacterial IN on precipitation at regional scales.

14/01706 Inverse prediction and optimization of flow control conditions for confined spaces using a CFD-based genetic algorithm

Xue, Y. *et al. Building and Environment*, 2013, 64, 77–84.

Optimizing an indoor flow pattern according to specific design goals requires systematic evaluation and prediction of the influences of critical flow control conditions such as flow inlet temperature and velocity. In order to identify the best flow control conditions, conventional approach simulates a large number of flow scenarios with different boundary conditions. This paper proposes a method that combines the genetic algorithm (GA) with computational fluid dynamics (CFD) technique, which can efficiently predict and optimize the flow inlet conditions with various objective functions. A coupled simulation platform based on GenOpt (GA program) and Fluent (CFD program) was developed, in which the GA was improved to reduce the required CFD simulations. A mixing convection case in a confined space was used to evaluate the performance of the developed program. The study shows that the method can predict accurately the inlet boundary conditions, with given controlling variable values in the space, with fewer CFD cases. The results reveal that the accuracy of inverse prediction is influenced by the error of CFD simulation that need be controlled within 15%. The study further used the predicted mean vote as the cost function to optimize the inlet boundary conditions (e.g. supply velocity, temperature, and angle) of the mixing convection case as well as two more realistic aircraft cabin cases. It presents interesting optimal correlations among those controlling parameters.

14/01707 Numerical simulation of oscillatory flows over a rippled bed by immersed boundary method

Shen, L. and Chan, E.-S. *Applied Ocean Research*, 2013, 43, 27–36.

In this paper, a well-developed numerical model based on the immersed boundary (IB) method is used to study oscillatory flows over a bed with large-amplitude ripples in a systematic manner. The work shows that the complex flow over the rippled bed can be

numerically dealt with in Cartesian coordinate by the IB method and that the IB method is able to provide main features of the flows near the ripples. An accurate simulation of vortices generation as a result of flow separation at the rippled bed is obtained. It is found that the oscillatory flows start to separate during the flow deceleration when the Keulegan–Carpenter number is small. The steady streaming for various ripple steepness is simulated and the criterion for separating the single and double structure streaming is also discussed. Moreover, a new type of steady streaming which consists of a pair of embedded recirculations in the vicinity of the ripple trough is obtained for relatively steep ripples in this work. The numerical results, including the steady streaming in particular, may be helpful to improve the understanding of the sediment transport and the seabed evolution with natural ripples under sea waves.

14/01708 One-dimensional N_2 gas inside single-walled carbon nanotubes

Kramberger, C. *et al. Carbon*, 2013, 55, 196–201.

The unexpected presence of a linear arrangement of co-axially oriented N_2 molecules inside aligned single-walled carbon nanotubes is revealed by high resolution near-edge X-ray absorption spectroscopy. The encapsulated N_2 molecules exhibit free stretching vibrations with a long electronic lifetime of the X-ray-excited anti-bonding π^* states. Molecular dynamics simulations confirm that narrow-diameter nanotubes ($d < 1$ nm) are crucial for stabilizing the linear arrangement of aligned N_2 molecules.

14/01709 Pre-equilibrium neutron-emission spectra of ^{238}U with an effective nucleon–nucleon interactions

Tel, E. *et al. Annals of Nuclear Energy*, 2013, 58, 12–18.

In this study, the initial exciton numbers for the target nucleus ^{238}U were calculated through a new method offered in an earlier study. Neutron-emission spectra produced by (n,xn) reactions on ^{238}U nuclei have been calculated by using Hartree–Fock method with effective nucleon–nucleon Skyrme interactions with SKM* parameters. Pre-equilibrium nuclear reactions have been used to investigate the effect of initial exciton numbers on the nucleon emission spectra. Calculations have been made in the framework of the hybrid, equilibrium and GDH models using ALICE/ASH computer code. The initial exciton numbers calculated with the theoretical neutron and proton densities have been obtained with SKM* for the ^{238}U(n,xn) reaction at 14.0 and 18.0 MeV incident neutron energies. The authors also compared the geometry-dependent hybrid model, newly evaluated with the initial exciton number calculations of the neutron emission spectra of the ^{238}U(n,xn) reaction. The obtained results are discussed and compared with the available experimental data and are shown to be in agreement with each other. All calculated results have been compared with experimental data from experimental nuclear reaction data.

14/01710 Quantum excitation spectrum of hydrogen adsorbed in nanoporous carbons observed by inelastic neutron scattering

Olsen, R. J. *et al. Carbon*, 2013, 58, 46–58.

Inelastic neutron scattering spectra have been collected over a wide range of momentum transfer from H_2 adsorbed in several high-porosity carbon substrates. The authors show theoretical spectra which consider the relationship between rotational and translational transitions in the highly anisotropic adsorption environment, proving that different rotational excitations contain different amount of recoil broadening and motivating a new analysis method which considers both types of transitions at once. Spectra for most of the samples, including two activated carbons, are very similar to one another, supporting models of nanoporous carbons which are quite similar on the sub-nanometre scale. The exception is the low-energy side of the rotational peak, indicating important differences in the initial distribution of motion. The authors also find more subtle differences in the spectra which may be linked to differences in sample heterogeneity and surface rugosity. One sample does have a very different spectrum, which is not explained by standard models of this system. They also observe a significantly reduced effective mass in the spectrum of recoil transitions and evidence of coupling of rotational and translational motion resulting from periodic variations in orientation of the rotational states.

14/01711 Simulation of neutron radiograph images at the neutron radiography reactor

Morgan, S. W. *et al. Annals of Nuclear Energy*, 2013, 57, 341–349.

The ability to accurately simulate potential radiographic images produced by a radiographic facility can improve the facility's ability to design experiments and evaluate images. The image simulation methods detailed in this paper predict the radiographic image of an object based on the foil reaction rate data obtained by placing a model of the object in front of the image plane in a Monte Carlo beamline model. The image simulation method utilizes a characteristic curve relating foil activity to optical density for the film and foil combination in use at the neutron radiography reactor. The simulation validation compared a radiograph of a polyethylene step block to a simulated radiograph of the same step block. The simulation accurately predicts the optical density in each region of a radiograph of the step block. The simulated radiograph predicts the average optical density of the actual radiograph more accurately for the thinner steps, resulting in step averaged optical density differences between the actual and simulated images of −11.6% for the thinnest step versus a difference of −34.7% for the thickest step, possibly due to the greater accuracy of the higher optical density region of the characteristic curve. Applying the scanner calibration curve to the calculated optical density values decreases the difference between the actual radiograph pixel values and the simulated pixel values for each step except the thinnest step. The step averaged differences between the corrected and actual images increase from −11.6% to −17.0% for the thinnest step and decrease from −34.7% to +7.7% for the thickest step after the calibration curve is applied.

14/01712 Technical aspects concerning the detection of animal waste nutrient content via its electrical characteristics

Bietresato, M. and Sartori, L. *Bioresource Technology*, 2013, 132, 127–136.

The variables that influence the corrosion of three metals (galvanized steel, stainless steel, brass) usable for a manure nutrient probe were examined, identifying the best material for field applications. The nutrients in 18 liquid manures were then estimated through the voltage drop between the terminals of a prototype probe. Response surface modelling gave the regression functions relating each investigated response only to the statistically significant factors. After 168 h in the manure, it was determined that: stainless steel was the most suitable material for very close electrodes (mass: −1.8% at 15 mm), brass can be used with any inter-electrode distance (mass: −13.0% maximum at 35 mm). The prototype probe gave reliable estimates ($R^2 \geq 0.744$) of N_{tot}, N_{amm}, P_{tot}, K_{tot} when dry matter and temperature were also accounted for in the regression analysis. Not considering dry matter but just electronically-detectable quantities (temperature, voltage drop), the estimates were only reliable ($R^2 \geq 0.656$) over 20 °C.

14/01713 The Diavik Waste Rock Project: implications of wind-induced gas transport

Chi, X. *et al. Applied Geochemistry*, 2013, 36, 246–255.

Wind-induced gas transport in a test-scale unsaturated waste rock pile was investigated at the Diavik diamond mine, Northwest Territories, Canada. Differential gas pressures were measured in 2008 at 49 locations within a field-scale experimental waste rock pile (test pile) and at 14 locations on the surface of the test pile at 1-min intervals. Wind speed and direction were measured at 10-min intervals and decomposed into north, south, east, and west vectors. Correlations between wind vectors and pressure measurements indicate that the wind influences pressure fluctuations in the test pile. The strength of the correlation is roughly inversely proportional to the distance between the measurement ports and the atmospheric boundary. The relationship between the magnitude of the wind vector and pressure fluctuations on the surface of the test pile is non-linear. However, the relationship between internal and surface pressure measurements is linear, suggesting that gas flow within the test pile follows Darcy's Law. Spectral analysis demonstrates that the dominant periods of the wind range from 1 to 14 d. A one-dimensional analytical solution to the flow equation is used to demonstrate that long periods have the most pronounced effect on transient gas flow within the test pile and that the penetration depth of the wind-induced gas pressure wave is a function of wind period and permeability of the test pile.

14/01714 Thermal optimisation of polymer extrusion using in-process monitoring techniques

Vera-Sorroche, J. *et al. Applied Thermal Engineering*, 2013, 53, (2), 405–413.

Polymer extrusion is an energy intensive process, which is often run at less than optimal conditions. The extrusion process consists of gradual melting of solid polymer by thermal conduction and viscous shearing between a rotating screw and a barrel; as such it is highly dependent on the frictional, thermal and rheological properties of the polymer. Extruder screw geometry and extrusion variables should ideally be tailored to suit the properties of individual polymers, but in practice this is rarely achieved due to the lack of understanding of the process. Here, in-process monitoring techniques have been used to characterize the thermal dynamics of the extrusion process. Novel thermocouple grid sensors have been used to measure melt temperature fields within flowing polymer melts at the entrance to an extruder die in conjunction with infra-red thermometers and real-time quantification of energy consumption. A commercial grade of polyethylene has been examined using three extruder screw geometries at different extrusion operating conditions to understand the process efficiency. Extruder screw

geometry, screw rotation speed and set temperature were found to have a significant effect on the thermal homogeneity of the melt and process energy consumed.

14/01715 Thermal pulse energy harvesting

McKay, I. S. and Wang, E. N. *Energy*, 2013, 57, 632–640.

This paper presents a new method to enhance thermal energy harvesting with pulsed heat transfer. By creating a phase shift between the hot and cold sides of an energy harvester, periodically pulsed heat flow can allow an available temperature gradient to be concentrated over a heat engine during each thermal pulse, rather than divided between the heat engine and a heat sink. This effect allows the energy harvester to work at maximum power and efficiency despite an otherwise unfavourable heat engine–heat sink thermal resistance ratio. In this paper, the analysis of a generalized energy harvester model and experiments with a mechanical thermal switch demonstrate how the pulse mode can improve the efficiency of a system with equal engine and heat sink thermal resistances by over 80%, although at reduced total power. At a 1 : 2 engine–sink resistance ratio, the improvement can simultaneously exceed 60% in power and 15% in efficiency. The thermal pulse strategy promises to enhance the efficiency and power density of a variety of systems that convert thermal energy, from waste heat harvesters to the radioisotope power systems on many spacecraft.

14/01716 Thermodynamic analysis of lead–bismuth eutectic turbulent flow in a straight tube

Guo, J. and Huai, X. *Energy*, 2013, 57, 600–606.

The entropy generation in lead–bismuth eutectic (LBE) turbulent flow in a cooled straight tube with a diameter of 10 mm and a length of 1 m is numerically investigated taking into account the temperature-dependent of LBE properties. The standard k-epsilon turbulence model combined with appropriate turbulence Prandtl number is adopted to describe the turbulent heat transfer and flow of LBE under different heat flux and flow conditions. The average cooling heat flux of 5×10^5 W/m^2, the flow inlet temperature of 723.15 K and the flow velocity of 1–3.5 m/s are used in these studies. The heat transfer entropy generation rate is far larger than frictional entropy generation rate, and the heat transfer entropy generation rate distributes more widely than frictional entropy generation over the flow cross-section. Under the same heat transfer area and heat load conditions, the thermodynamic performance of the LBE flow under considered conditions is the best under a slight increase of the absolute heat flux along flow direction condition, followed by the constant heat flux condition; the decreasing absolute heat flux along flow direction is the worst.

Fuel cell technology

14/01717 A sandwich structured membrane for direct methanol fuel cells operating with neat methanol

Wu, Q. X. *et al. Applied Energy*, 2013, 106, 301–306.

Water starvation at the anode represents a challenging issue in the development of direct methanol fuel cells (DMFCs) operating with neat methanol. To tackle the issue, a multi-layered membrane, consisting of an ultra-thin reaction layer sandwiched between two thin membranes, is proposed and developed. The reaction layer is composed of well-dispersed PtRu catalysts, SiO_2 nanoparticles and Nafion ionomers. During the fuel cell operation, the methanol permeated from the anode catalyst layer and the oxygen permeated from the cathode catalyst layer meet and react in the reaction layer of the sandwich structured membrane to form water and CO_2. The produced water is then maintained at a relatively high level by the hygroscopic SiO_2 nanoparticles in the sandwich structured membrane. As a result, such a created water source at a high concentration level can supply the water required not only for the anode methanol oxidation reaction but also for membrane hydration. The performance characterization demonstrates that the DMFC with the sandwich structured membrane results in much higher performance than that with a single layer Nafion membrane does.

14/01718 Calcined polyaniline–iron composite as a high efficient cathodic catalyst in microbial fuel cells

Lai, B. *et al. Bioresource Technology*, 2013, 131, 321–324.

A new type of carbon–nitrogen–metal catalyst, PANI–Fe–C, was synthesized by calcination process. According to the results of FT-IR and XPS analysis, polyaniline chain was broken by calcination. Small nitrogen-contained molecular fragments were gasified during calcination process, while the remaining nitrogen atoms were enchased in the new produced multiple carbon rings by C–N and C=N bonds and performed as the catalytic active sites and the covalent centres for soluble iron components. Calculated from the polarization curves, a maximum power density of 10.17 W/m^3 for the MFC with the synthetic catalyst was obtained, which was slightly higher than the MFC with Pt/C catalyst of 9.56 W/m^3. All the results obtained in this paper proved that the newly synthetic nitrogen–carbon–metal catalyst would be a potential alternative to the expensive Pt/C catalyst in the field of MFC.

14/01719 Calculation of the energy efficiency of fuel processor – PEM (proton exchange membrane) fuel cell systems from fuel elementar composition and heating value

Salemme, L. *et al. Energy*, 2013, 57, 368–374.

This simulative work analyses the impact of fuel type on the energy efficiency of systems composed by a fuel processor for hydrogen production and a proton exchange membrane fuel cell. Two fuel processors are simulated, one employs steam reforming to produce hydrogen, the other one autothermal reforming. In both cases, fuel processing is completed by two water gas shift units and one preferential CO oxidation unit. Five classes of fuels are considered, i.e. alkanes, alkenes and alkynes, alcohols and aromatics and steam to carbon and oxygen to carbon inlet ratios, reforming temperature, fuel cell split fraction and exhaust gas temperature are explored as operative parameters. For each fuel considered, Aspen Plus® was used to calculate the operative conditions that maximize the energy efficiency of the systems. For each system, the data were employed to identify an analytic expression to calculate the best possible energy efficiency given the elementar composition of the fuel and its lower heating value. The expressions proved to hold true for a broad range of fuel types.

14/01720 Durability and degradation mechanism of titanium nitride based electrocatalysts for PEM (proton exchange membrane) fuel cell applications

Avasarala, B. and Haldar, P. *Energy*, 2013, 57, 545–553.

Titanium nitride (TiN) is a promising material that has a higher potential for increasing electrocatalyst durability in proton exchange membrane (PEM) fuel cells. This study provides an explanation for the higher catalytic performance of titanium nitride nanoparticles (TiN NP)-based electrocatalyst (Pt/TiN) when compared to that of Pt/C, using X-ray photoelectron spectroscopy. The authors also compare its durability with that of the conventional Pt/C electrocatalyst and explain its degradation mechanism under fuel cell conditions. Unlike Pt/C which degrades significantly via the Pt agglomeration and carbon support corrosion mechanisms, the authors show that Pt/TiN degrades predominantly via Pt agglomeration mechanism. TiN has a higher resistance to corrosion than carbon under electrochemical conditions; as a result catalyst support corrosion mechanism plays a minor role in the degradation of Pt/TiN. For a given mass and particle diameter, TiN has a higher number of catalyst support particles than carbon due its higher material density. As a result it is hypothesized that, for the same amount of catalyst loading on both supports, the Pt/TiN has a higher Pt particle density on its surface compared to Pt/C and can result in a faster rate of Pt particle agglomeration during the electrocatalyst degradation. This hypothesis is tested theoretically by calculating the support to catalyst particle ratio. It is observed that the support to catalyst particle ratio is 1 : 21 for 20 wt% Pt/C and 1 : 60 for 20 wt% Pt/TiN. The hypothesis is also tested experimentally by two different methods, the first of which is by measuring and comparing the Pt particle sizes after subjecting the Pt/TiN and Pt/C to accelerated durability tests (ADT: 0–1.3 V RHE (reversible hydrogen electrode), 1100 cyc). Secondly, the Pt particle density on the electrocatalysts is changed by varying the amount of Pt loading (10 and 30 wt%) and the Pt particle size is measured at the end of ADT. Both methods lead to the same conclusion that Pt/TiN has a significantly higher Pt particle size at the end of ADT (compared to Pt/C) indicating towards its increased rate of Pt agglomeration mechanism. Furthermore, a new approach is suggested where the oxynitride layer is grown on Pt/TiN resulting in partial encapsulation of Pt particles on the surface of TiN catalyst support thereby reducing the Pt agglomeration during fuel cell operation.

14/01721 Ejector design and performance evaluation for recirculation of anode gas in a micro combined heat and power systems based on solid oxide fuel cell

Vincenzo, L. *et al. Applied Thermal Engineering*, 2013, 54, (1), 26–34.

In this paper, a theoretical analysis of an ejector for micro combined heat and power systems based on solid oxide fuel cell (SOFC) system for small-scale residential applications is presented. A novel detailed procedure for the ejector designing is provided and its effectiveness is validated through a comparison with testing results. The ejector geometry is analysed in terms of component efficiency. The SOFC system performance with regard the recirculation of anode gas is finally discussed. Results show that fuel inlet temperature and the diameter of the ejector mixing chamber of the ejector largely affect the ejector performance. A large mixing chamber diameter allows a high entrainment ratio but causes a worse ejector efficiency suggesting a highest efficiency still ensuring the required entrainment ratio. At system level, it is shown that the degree of fuel pre-reforming affects the recirculation ratio. Besides, if anode gas recirculation is implemented the system capital cost decreases due to reduction in

size of ancillary components. The high electrical efficiency achieved by the system reduces the heat output and makes it more attractive when less heat is demanded.

14/01722 Operation and characterization of a microbial fuel cell fed with pretreated cheese whey at different organic loads

Tremouli, A. *et al. Bioresource Technology*, 2013, 131, 380–389.
Electricity production from filter sterilized cheese whey at different organic loads (0.35, 0.7, 1.5, 2.7 and 6.7 g COD/L) was investigated in a two-chamber microbial fuel cell (MFC). The best performance of the cell was observed at the highest concentration of the pretreated (filter sterilized) cheese whey (6.7 g COD/L) corresponding to a maximum power density of approximately 46 mW/m^2. Experiments using glucose (0.35 g COD/L) were also performed for comparison reasons. The study of the open-circuit impedance characteristics of the MFC and of the individual electrodes revealed that the open-circuit impedance of the MFC depended to practically the same extent on both the ohmic resistance between the anode and cathode and the overall polarization resistance. The polarization resistance of the MFC decreased significantly under closed-circuit conditions, which in turn implies that the ohmic overpotential is the main contribution to the energy losses in two-chamber MFCs.

14/01723 Optimization of parameters for hot-pressing manufacture of membrane electrode assembly for PEM (polymer electrolyte membrane fuel cells) fuel cell

Okur, O. *et al. Energy*, 2013, 57, 574–580.
In this study, optimization of the hot-pressing parameters in manufacturing of the membrane electrode assembly (MEA) is carried out using response surface method (RSM). The important parameters to be optimized in the MEA production are temperature, pressure and the processing (pressing) time. Therefore, the studied temperature, pressure and pressing time intervals are 80–130 °C, 10–100 kg cm^{-2}, and 1–5 min, respectively. In the RSM, the objective function to be maximized is power density, whereas temperature, pressure and pressing time are all independent variables. This method generates a non-linear quadratic equation in terms of independent parameters. Based on contour plots and variance analysis, two optimum operation conditions are determined with respect to maximum power densities. In the first case; where the manufacturing cost and difficulties in operating conditions are taken into account, maximum power density is 862 mW cm^{-2} at the manufacture parameters of 97 °C, 66 kg cm^{-2} and 3.6 min. In the second case; where temperature, pressure and hot-pressing time are set to minimum values in order to save energy and manufacturing time, maximum power density of 768 mW cm^{-2} is achieved at 87 °C, 48 kg cm^{-2} and 1.15 min.

14/01724 Performance evaluation of a solid oxide fuel cell coupled to an external biogas tri-reforming process

Lo Faro, M. *et al. Fuel Processing Technology*, 2013, 115, 238–245.
This study deals with an investigation of the performance of a biogas-fed solid oxide fuel cell (SOFC) operating in combination with an external tri-reforming system. The tri-reforming process is carried out using a ceria supported Ni catalyst (1.75-wt% Ni/CeO_2), prepared by combustion synthesis. The catalytic tests are carried out at 800 °C with fixed CH_4/CO_2 molar ratio. Different O_2/CH_4 and H_2O/CH_4 molar ratios are investigated to evaluate the influence of different feed compositions on the performance of the integrated SOFC and tri-reforming system. The SOFC can tolerate different percentages of CO, CH_4 and CO_2 in the reformate stream without the need of steam addition. However, the SOFC performance varies consistently with the different reformate compositions; this effect is strongly related to the tri-reforming catalyst performance. The results indicate that the process using biogas tri-reforming and SOFC is promising for application in small and medium sized stationary power systems.

14/01725 Reactivity between carbon cathode materials and electrolyte based on industrial and laboratory data

Chauke, L. and Garbers-Craig, A. M. *Carbon*, 2013, 58, 40–45.
Interaction between electrolyte and carbon cathodes during the electrolytic production of aluminium decreases cell life. This paper describes the interaction between carbon cathode materials and electrolyte, based on industrial and laboratory data. It also reports on the degree of expansion of semi-graphitic and graphitized materials when exposed to a sodium rich environment. Phase relations in the slow cooled bath electrolyte, spent industrial cathodes and laboratory scale cathode samples were similar: all contained Na_3AlF_6, NaF, CaF_2 and $NaAl_{11}O_{17}$. Al_4C_3, AlN and NaCN were only detected in the spent industrial cathodes. The inability to locate Al_4C_3 in the laboratory scale samples could be due to very low concentrations of Al_4C_3 which could not be detected by X-ray diffraction (XRD), or to the limited direct contact between the produced aluminium and carbon material. XRD analysis confirmed that sodium intercalation into graphite did not take place. Wear of the examined carbon cathodes proceeded due to penetration of electrolyte and sodium into the cathode, followed by reactions with carbon and N_2 whereby AlN and NaCN formed. Once electrolysis started the carbon cathodes expanded rapidly, but slowed down after approximately an hour. Sodium expansion decreased with degree of graphitization of the carbon cathode material.

14/01726 Saline catholytes as alternatives to phosphate buffers in microbial fuel cells

Ahn, Y. and Logan, B. E. *Bioresource Technology*, 2013, 132, 436–439.
Highly saline solutions were examined as alternatives to chemical buffers in microbial fuel cells (MFCs). The performance of two-chamber MFCs with different concentrations of saline solutions in the cathode chamber was compared to those with a buffered catholyte (50 mM PBS). The use of a NaCl catholyte improved the CE to 43–60% (28% with no membrane) due to a reduction in oxygen transfer into the anolyte. The saline catholyte also reduced the membrane and solution resistance to 23 Ω (41 Ω without a membrane). The maximum power density of 491 mW/m^2 (240 mM NaCl) was only 17% less than the MFC with 50 mM PBS. The decrease in power output with highest salinity was due to reduced proton transfer due to the ion exchange membrane, and pH changes in the two solutions. These results show that MFC performance can be improved by using a saline catholyte without pH control.

14/01727 The impact of monochromatic blue and red LED light upon performance of photo microbial fuel cells (PMFCs) using *Chlamydomonas reinhardtii transformation* F5 as biocatalyst

Lan, J. C.-W. *et al. Biochemical Engineering Journal*, 2013, 78, 39–43.
Photosynthetic microbial fuel cells (PMFCs) are devices that convert chemical energy into electricity through the catalytic activity of photosynthetic microorganisms. Power densities produced by the photosynthetic microalgae depend on light sources and light intensities as these two factors can affect the chlorophyll formation, photosynthesis processes and stomata opening in the microalgae cells. In this study, *Chlamydomonas reinhardtii transformation* F5 was used as biocatalyst in photomicrobial fuel cells (PMFCs) and was illuminated with monochromatic blue and red lights at various intensities (100, 300, 600 and 900 lx). Kinetic analysis was used to describe the intracellular and extracellular electron transfer mechanism of the cells. The results demonstrate that the performance of PMFCs increased in terms of maximum power density and exchange current density (i_o) with the tendency of decreasing in internal resistance (R_{int}) and overpotential (η) values as increasing monochromatic blue and red light intensities. However, the PMFCs performed better under red light as compared to operating under blue light. The maximum power density can reach 12.947 mW m^{-2}, which could be a potential micro-power supply.

14/01728 The modeling of gold recovery from tetrachloroaurate wastewater using a microbial fuel cell

Choi, C. and Hu, N. *Bioresource Technology*, 2013, 133, 589–598.
In this study, tetrachloroaurate as an electron acceptor of a microbial fuel cell (MFC) has been studied to discover the parameters that affect the cost-effective recovery of gold. The modelling and equations for calculating the maximum actual efficiency and electrochemical impedance spectroscopic internal resistance of the MFC were also developed. The maximum power density (P_{max}) of 6.58 W/m^2 with a fill factor of 0.717 was achieved for 60 mL volumes of 2000 ppm Au(III) catholyte and 12.2 mM acetate anolyte, respectively. The P_{max} can also be predicted simply by measuring R_{int} by EIS. Additionally, the maximum actual MFC efficiency of about 57% was achieved, and the recovery efficiency of Au and the remaining concentration reached 99.89 ± 0.00% and 0.22 ± 0.00 ppm, respectively, for an Au(III) concentration of 200 ppm. The anodic concentration polarization quenching of the MFC strongly supports a mediator mechanism for the electron transfer from the microorganism to the anode.

15 ENVIRONMENT

Pollution, health protection, applications

14/01729 A critical assessment of global uranium resources, including uranium in phosphate rocks, and the possible impact of uranium shortages on nuclear power fleets

Gabriel, S. *et al. Annals of Nuclear Energy*, 2013, 58, 213–220.

Future energy demand scenarios elaborated by international organizations tend to be ambitious in terms of the installed nuclear power capacity, particularly when trying to absorb the effects of a growing world population, to account for gross domestic products and to curb greenhouse gas emissions. Current light water reactors use thermal neutrons and burn uranium (a natural, finite resource), whereas some future Generation IV reactors using fast neutrons (starting with an initial fissile load) will be capable of recycling their own plutonium and already-extracted depleted uranium (self-sufficient or breeder fast reactors). The availability of uranium therefore has a direct impact on the capacity of the reactors that can be built. It is therefore important to have an accurate estimate of the available uranium resources in order to plan for the world's future nuclear reactor fleet. This paper discusses the correspondence between the resources (uranium and plutonium) and the nuclear power demand as estimated by various international organizations. Furthermore, the estimate of how much uranium can be recovered from phosphate rocks is questioned and the impact of the downscaled estimate on the deployment of a nuclear fleet is assessed accordingly.

14/01730 Analysis of surface contributions to external doses in a radioactively contaminated urban environment designed by the EMRAS-2 Urban Areas Working Group

Hwang, W. T. *et al. Annals of Nuclear Energy*, 2013, 57, 179–184.

The EMRAS-2 Urban Areas Working Group, which is supported by the IAEA, has designed a variety of accidental scenarios to test and improve the capabilities of the models used for an evaluation of radioactive contamination in an urban environment. A variety of models including a Korean model, METRO-K, are used for predictive results on the hypothetical scenarios. This paper describes the predictive results of METRO-K for the hypothetical scenarios designed in the Working Group. The external dose resulting from the air contamination of Co-60 was evaluated, and its contribution was analysed with time as a function of the location of a receptor and precipitation conditions at the time of the contamination event. As a result, the external doses showed a distinctive difference with the locations to be evaluated and the precipitation conditions. Moreover, the contribution of contaminated surfaces for external doses was strongly dependent on the locations to be evaluated and the precipitation conditions. These results will provide essential information to assist the decision-making of appropriate countermeasures in an emergency situation of a radioactively contaminated urban environment.

14/01731 Assessment of human exposure level to PM_{10} in China

An, X. *et al. Atmospheric Environment*, 2013, 70, 376–386.

Epidemiological studies have found that atmospheric particulate matter, especially PM_{10} (inhalable particulate matter with aerodynamic diameter less than or equal to 10 μm) is one of the pollutants that are harmful to human health. In recent years, particulate matter pollution in China is becoming increasingly serious and PM_{10} has become the primary pollutant in Beijing and other cities. Therefore, it is necessary to carry out studies and a health damage assessment of PM_{10}. In human health damage assessment, measuring human exposure level to PM_{10} is required and crucial to provide accurate exposure data for the exposure–response relationship, and also for the accurate quantitative assessment of human exposure. The spatial distribution of particle concentration in China is variable because of spatial differences in the local economic level and the geographical environment. Along with the accelerating urbanization in China, city population density is high, and the population distribution is variable between and within cities, thus resulting in different population numbers exposed to different concentration ranges. Therefore, an accurate assessment of China's level of exposure to particulate matter is a priority and the basis for assessing the damage to public health caused by particle pollution. Using high accuracy population and PM_{10} monitoring data, this study analysed the human exposure to PM_{10} in different regions and typical cities of China. The results show that for most areas of China, the population-weighted PM_{10} exposure concentration is slightly higher than the annual mean concentration, meaning that more of the population is exposed to high concentrations, and most of the population is exposed to levels that meet the second national standard (between 40 and 100 $\mu g\,m^{-3}$), occupying about 83.7% of population and 76.3% of area in China. The population exposure to PM_{10} is higher in two types of typical regions and cities: areas with dense human populations such as Jingjinji, Beijing and Tianjin, and areas with more sand dust and factories such as the north-west and Chongqing.

14/01732 Atmospheric environmental impact assessment of a combined district heating system

Wang, H. *et al. Building and Environment*, 2013, 64, 200–212.

Assessing the atmospheric environmental impacts of district heating (DH) systems is of increasing importance as the environmental concerns and the eco-sustainability concept is more and more widespread in the energy sector around the world. However, this issue has been overlooked to some extent for past decades in China, which led to inappropriate assessments only by measuring pollutant emissions per unit floor area or unit heat supply. This paper presents an atmospheric environmental assessment model incorporating the state of the art AERMOD modelling and the concept of normalized population distribution weights (NPDWs) to compute the mean spatial distribution (MSD) of pollutants for qualitatively evaluating the atmospheric environmental impacts of DH. The authors demonstrate the model in assessing different heating scenarios, characterized by basic heat load ratio in a real-life combined district heating system of Daqing city with a population of 2.7 million people. The results show that the presented model and MSD concentrations furnish a better base to assess the atmospheric environmental impact. The authors also show how the combined district heating system can undertake a part of CO_2 emission reduction burden in the DH sector at a city-scale.

14/01733 Critical loads and H^+ budgets of forest soils affected by air pollution from oil sands mining in Alberta, Canada

Jung, K. *et al. Atmospheric Environment*, 2013, 69, 56–64.

The authors investigated the critical load (CL) and exceedance (EX) of sulfur (S) deposition, temporal changes in soil chemistry, and H^+ budget of soils in plots dominated by *Pinus banksiana* (jack pine) or *Populus tremuloides* (trembling aspen, aspen) in two acid-sensitive watersheds to assess the risk of soil acidification by S emissions from oil sands mining in the Athabasca oil sands region (AOSR), Canada. The CLs and EXs were determined by two methods: one was based on bulk deposition and the other based on total deposition (as a sum of bulk deposition and interception deposition). The CLs ranged from 223 to 711 $mol_c\,ha^{-1}\,yr^{-1}$ based on bulk deposition. Those values were similar to that obtained based on total deposition. However, EXs based on bulk deposition were significantly lower ($p < 0.001$) than those based on total deposition due to the relative increase of SO_4^{2-} concentrations in interception deposition, indicating that EXs based on bulk deposition only could underestimate the risk of soil acidification in the AOSR. The S deposition did not exceed CLs in the long term for both methods. The pH in the forest floor increased and available SO_4^{2-} (as the sum of soluble and adsorbed SO_4^{2-}) in the forest floor and surface mineral soils increased in both jack pine and aspen stands between 2005 and 2010. The H^+ budget ranged from −289 to −130 $mol_c\,ha^{-1}\,yr^{-1}$ in jack pine stands and from −510 to −371 $mol_c\,ha^{-1}\,yr^{-1}$ in aspen stands. The results suggest that (1) soils in the studied forest stands have recovered from acidification based on the increasing soil pH over time and the negative H^+ budget, and (2) the risk of soil acidification should be assessed by CL and EX calculated based on total deposition.

14/01734 Directions in green roof research: a bibliometric study

Blank, L. *et al. Building and Environment*, 2013, 66, 23–28.

Green roof research is a multidisciplinary and new research area. The authors conducted a bibliometric quantification to assess the rate of publications in specific areas of research for this novel research area based on the scientific literature as available from the Web of Science. Bibliometric research can provide valuable information about changes in the trends within a particular area of research. For example, the authors found that the number of publications in this field increased in the last two decades at very similar pace to other pre-established academic disciplines. They also found that papers on green roofs were classified into 32 research areas. There was very little change in the frequency of most research areas through time. The percentages of plant sciences, forestry, marine and freshwater biology and biodiversity conservation of the total research areas classifications used each year increased significantly with time, while architecture decreased significantly with time signifying an increased interest in environmental issues and less focus on architectural issues. The distribution of publications between countries has been skewed, with the USA and the European Union conducting 66% of the research, and thus allocation of research effort is focused in those continents and predominantly in temperate ecosystems. However, there has been a sharp increase in the number of countries that conduct green roof research. This work provides a suite of indicators that can be combined to give a useful picture of the development of green roof research and identifies the challenges which lie ahead for this novel research area.

14/01735 Does the rapid development of China's urban residential buildings matter for the environment?

He, X. *et al. Building and Environment*, 2013, 64, 130–137.

The exponential development of the urban real estate sector has become one of the main forces behind the development of China's urban economy. The massive development of urban buildings, however, aggregates domestic environmental pressures. This study develops a four-quadrant matrix to elaborate the direct and indirect impacts on the construction and operation of urban residential buildings and

applies a hybrid life cycle assessment method to quantify the overall impacts. The results show that the total energy consumption, water consumption, chemical oxygen demand, ammonia nitrogen (NH_3–N), sulfur dioxide (SO_2), and nitrogen oxides (NO_x) emissions of the overall life span of the urban residential buildings accounted for 5.4%, 5.6%, 3.0%, 3.5%, 3.9% and 4.0%, respectively, of the national total in 2010. The indirect productive impacts accounted for 76.2% of the energy consumption, 86.4% of the water consumption, and 81.6% of the air pollution emission in 2010. With respect to the potential mitigation alternatives in the next 5 years, a scenario analysis suggests that a moderate slow-down of the construction of new buildings should be the highest priority, and promoting the application of greener housing materials and more advanced construction techniques should also be considered.

14/01736 Driving carbon reduction strategies adoption in the Australian construction sector – the moderating role of organizational culture

Wong, P. S. P. and Zapantis, J. *Building and Environment*, 2013, 66, 120–130.

In recent years, numbers of strategies were advocated to foster carbon reduction in built environment. However, few studies have acknowledged that strategies adoption is a matter of organizational culture (OC). In this study, a conceptual model that depicts the hypothesized relationship among carbon reduction drivers, strategies adoption and OC is developed. The model is then tested with data collected via a survey conducted in Australia. The results suggest that the significant relationship between the carbon tax and the adoption of carbon reduction strategies can be further enhanced by OC in terms of goal clarity, rewards, and innovation. Surprisingly, stringent regulations may not necessarily induce adoption of carbon reduction strategies in built environment even if OC exists.

14/01737 Field studies on human thermal comfort – an overview

Kumar Mishra, A. and Ramgopal, M. *Building and Environment*, 2013, 64, 94–106.

This paper presents an exhaustive overview of the field studies carried out in the past few decades on human thermal comfort. To get a better grasp of patterns in observed data and to facilitate comparison across investigations, the thermal comfort field studies are grouped using the Köppen–Geiger climatic classification of their locations. Effects of relevant environmental, physiological, and other aspects that can have an effect on thermal comfort are reviewed and discussed. Field studies across the board show that people have considerable capacity to adapt to their surroundings provided they have sufficient adaptive opportunities. This observation holds good for both air-conditioned as well as free running buildings. However, studies show that conditioned spaces have narrower comfort zones compared to free running buildings. Across climatic zones, most popular means of adaptation are related to the modification of air movement and clothing. The ease, economy, and effectiveness of adaptive opportunities play a major role in occupants' adaptation to the surroundings. Studies show that individuals are likely to perceive the same thermal environment differently and environments lacking adaptive avenues normally receive poor comfort ratings. Studies also indicate that for adaptive comfort equations, the running mean temperature may be a better outdoor index compared to the monthly mean temperature.

14/01738 Impact of building materials on indoor formaldehyde levels: effect of ceiling tiles, mineral fiber insulation and gypsum board

Gunschera, J. *et al. Building and Environment*, 2013, 64, 138–145.

Materials such as building products or furnishings present in climatically controlled or uncontrolled indoor environments significantly influence the indoor air quality (IAQ). In this study, the contribution of formaldehyde emissions from building materials and influences of adsorption/desorption behaviour to indoor air pollution is investigated in a custom-made test house environment, located in a climate-controlled 48 m^3 stainless-steel chamber. The complete test house study comprised three experimental cycles applying different types of ceiling tiles as target building materials. In each cycle one type of ceiling tile was used, while the housing construction and fittings were left unchanged. One cycle was divided into three steps to differentiate the contribution of each material to the overall IAQ: after the background monitoring of the empty housing frame (step I), ceiling tiles were installed in the house and the air quality was monitored for one week (step II). Finally, furniture and carpet were introduced into the house and the air was again monitored for one week (step III). Additionally, gypsum boards and ceiling tiles were characterized by determination of their emission, diffusion and adsorption/desorption rates with regard to formaldehyde. It is the most important finding of this study that the resulting formaldehyde concentration does not simply result from additive emissions from the materials involved. In fact, it can only be explained accurately when taking into account multiple parameters.

14/01739 Migration of sediment deposition due to the construction of large-scale structures in Changjiang Estuary

Ma, G. *et al. Applied Ocean Research*, 2013, 43, 148–156.

The paper presents measurements of sediment deposition in the navigation channel of Changjiang Estuary during the construction of the world largest jetty-spur system. A significant change of sediment deposition pattern is found after the second stage of the project, which extended the previous 25 km long jetties built in the first stage to about 50 km. The measurements show that the main deposition region migrated from the lower reach to upper reach of the navigation channel, with the strongest deposition occurred at the upper middle reach. The physical mechanisms inducing the migration of the sediment deposition region are studied numerically using the finite-volume coastal ocean model. Model results reveal that the tidal currents as well as the sediment processes in the northern passage are greatly changed by the structures. With the extension of the structures, suspended sediment concentration decreases at the upper reach and increases at the lower reach, resulting in a seaward migration of turbidity maximum in the northern passage. The changes of suspended sediment concentration distributions are mainly caused by the adjustments of tidal currents at ebb. The analysis based on the local momentum balance identifies two mechanisms causing these adjustments.

14/01740 Monte Carlo calculations for gamma-ray mass attenuation coefficients of some soil samples

Tarim, U. A. *et al. Annals of Nuclear Energy*, 2013, 58, 198–201.

The authors developed a simple Monte Carlo code to determine the mass attenuation coefficients of some soil samples at nine different gamma-ray energies (59.5, 80.9, 122.1, 159.0, 356.5, 511.0, 661.6, 1173.2 and 1332.5 keV). Results of the Monte Carlo calculations have been compared with tabulations based upon the results of photon cross-section database and with experimental results by other researchers for the same samples. The calculated mass attenuation coefficients were found to be very close to the theoretical values and the experimental results.

14/01741 Multi-objective methods for determining optimal ventilation rates in dwellings

Das, P. *et al. Building and Environment*, 2013, 66, 72–81.

The optimal ventilation rate in a dwelling is a trade-off between the requirement to minimize ventilation heat losses to help meet national greenhouse gas emission targets and the need to minimize adverse health impacts arising from exposure to cold temperatures and pollutants from indoor and outdoor origin. This paper presents approaches for exploring these trade-offs based on two implementations of multi-objective optimization that consider both energy efficiency and health impacts. Both methods aggregate the various performance criteria into a single criterion, but the first method monetizes the performance criteria, while the second method weights them in a more general way. Unlike in the monetization approach, the generalized multi-objective optimization approach is found to be robust against scaling of the health impacts and energy savings that is independent of the ventilation rate. As a result it is less sensitive to assumptions made in the models regarding heating system efficiency, absolute health burden level, and dwelling occupancy. It is however sensitive to assumptions regarding pollutant production rates and balance-point temperatures, which affect health impacts and energy savings in a way correlated with ventilation rate. A preliminary application of the methods to a typical UK flat and detached house finds that the optimal ventilation rate may vary with built form. Application of the generalized multi-objective optimization approach in which health impacts and energy savings are equally weighted, suggests an optimal annual average air change rate of 0.4/h for the detached house, and 0.7/h for the flat.

14/01742 National survey of summertime temperatures and overheating risk in English homes

Beizaee, A. *et al. Building and Environment*, 2013, 65, 1–17.

This paper presents one of the first national scale studies of summertime temperatures in English dwellings. Living room and bedroom temperatures were recorded in 207 homes across the England during the cool summer of 2007. Data were also collected by face-to-face household interviews. Fourteen homes (7%) were observed to be heated for part or all of the analysis period (July to August). Based on the BSEN15251 adaptive thermal comfort model, the 193 free-running dwellings would, in general, to be considered as uncomfortably cool. Over 72% of living rooms and bedrooms had more than 5% of hours below the BSEN15251 Cat II lower threshold, with over 50% having more than 5% of hours below the Cat III threshold. Detached homes and those built before 1919 were significantly cooler ($p < 0.05$) than those of other type and age. Static criteria revealed that, despite the cool summer, 21% of the bedrooms had more than 5% of night-time

hours over 26 °C; which is a recommended upper limit for bedrooms. The bedrooms of modern homes, i.e. those built after 1990 or with cavity walls, were significantly warmer ($p < 0.05$). The bedrooms in homes built prior to 1919 were significantly cooler ($p < 0.05$). The living rooms of flats were significantly warmer than the living rooms in the other dwelling types ($p < 0.05$). The incidence of warm bedrooms in modern homes, even during a cool summer, is of concern, especially as there is a strong trend towards even better insulation standards in new homes and the energy-efficient retrofitting of existing homes.

14/01743 Public attitudes to climate change and carbon mitigation – implications for energy-associated behaviours

von Borgstede, C. *et al*. *Energy Policy*, 2013, 57, 182–193.

This work explores public opinions regarding climate change and mitigation options and examines how psychological factors, such as attitudes, norms, and willingness to pay, determine self-reported energy-efficient behaviour. The aim is to create knowledge for the design and implementation of policy measures. The results of an opinion poll conducted in 2005 and 2010 are compared. The number of respondents favouring new technologies as a way to reduce emissions was substantially lower in 2010 than in 2005, whereas there was an increase in the number of people who acknowledged that lifestyle changes are necessary to counteract climate changes. This indicates an increased awareness among the public of the need for lifestyle changes, which could facilitate implementation of policies promoting environmental behaviour. Renewable energy and energy saving measures were ranked as the top two measures for mitigating climate change in both polls. In determining which energy behaviours of the public are determined by psychological factors, an analysis of the 2010 survey revealed that respondents with pro-environmental attitudes towards global warming favour significantly increased use of renewable energy technologies and greater engagement in energy-efficient behaviours.

14/01744 Relating five bounded environmental problems to China's household consumption in 2011–2015

Liu, L.-C. and Wu, G. *Energy*, 2013, 57, 427–433.

With the rapid development of industrialization and urbanization, China faces a number of serious environmental problems that significantly affect economic and social sustainable development. This study quantifies the CO_2, SO_2, NO_x, chemical oxygen demand (COD) and ammonia–nitrogen emissions resulting from household consumption, based on an input–output model used to identify which consumption items appear mainly responsible for environmental impacts and which consumption items can lead to different environmental impacts in 2007. Using a 2007 input–output table, the authors found that CO_2, SO_2, COD, NO_x, and ammonia–nitrogen emissions from household consumption in 2007 accounted for approximately 42.17%, 33.67%, 33.11%, 28.83% and 30.38% of China's total emissions, respectively. Each environmental impact arises from the consumption of a mix of goods and services. 'Agriculture' and 'food and tobacco manufacture' consumption contributed more than 50% of COD and ammonia nitrogen emissions; 'electricity and heating generation' and 'food and tobacco manufacture' accounted for more than 50% of SO_2, NO_x and CO_2 emissions. Consumption items are classified into different types, with types 1 and 3 countering each other, illustrating a trade-off between stimulating household consumption, mitigating COD and ammonia–nitrogen emissions and mitigating CO_2, SO_2 and NO_x emissions.

14/01745 Remotely sensed thermal pollution and its relationship with energy consumption and industry in a rapidly urbanizing Chinese city

Zhao, X. *et al*. *Energy Policy*, 2013, 57, 398–406.

Taking the city of Xiamen, China, as an example, this study used thermal infrared remote sensing to detect thermal pollution, and examined its relationship to energy consumption and the industrial economy. Monthly changes in 2002 and dynamics throughout the period of rapid urbanization (1987–2007) are analysed. It is found that seasonal variation led to distinct shapes and sizes of thermal pollution areas, and winter thermal pollution was highly indicative of industrial and energy transformation sources. Industrial enterprises were the dominant sources of winter thermal pollution in Xiamen. The number and ratio of industrial thermal pollution sources increased stably in the earlier years, and dramatically in the later period (2002–2007), attributable to the effects of China entering the World Trade Organization. Linear regression shows that the number of thermal pollution sources was strongly correlated with several factors of the industrial economy and energy consumption, including industrial outputs, industrial enterprise numbers, liquid petroleum gas and electricity. Related mitigation measures are also discussed. This research builds a link between remote sensing-detected thermal pollution information and statistical energy consumption data, as well as industrial economy statistics. It thereby enhances understanding of the relationship between urbanization, industrialization, energy consumption and related environmental effects.

14/01746 Road vehicle emission factors development: a review

Franco, V. *et al*. *Atmospheric Environment*, 2013, 70, 84–97.

Pollutant emissions need to be accurately estimated to ensure that air quality plans are designed and implemented appropriately. Emission factors (EFs) are empirical functional relations between pollutant emissions and the activity that causes them. In this review article, the techniques used to measure road vehicle emissions are examined in relation to the development of EFs found in emission models used to produce emission inventories. The emission measurement techniques covered include those most widely used for road vehicle emissions data collection, namely chassis and engine dynamometer measurements, remote sensing, road tunnel studies and portable emission measurements systems. The main advantages and disadvantages of each method with regards to emissions modelling are presented. A review of the ways in which EFs may be derived from test data is also performed, with a clear distinction between data obtained under controlled conditions (engine and chassis dynamometer measurements using standard driving cycles) and measurements under real-world operation.

14/01747 The Diavik waste rock project: water flow through mine waste rock in a permafrost terrain

Neuner, M. *et al*. *Applied Geochemistry*, 2013, 36, 222–233.

A field experiment is being carried out at the Diavik diamond mine in northern Canada to investigate the influence of unsaturated flow behaviour on the quality of drainage from mine waste rock piles in a region of continuous permafrost. This paper is part of a series describing processes affecting the weathering of waste rock and transport of reaction products at this site; here the focus is on unsaturated water flow and its role in mass loading. Two 15 m-high instrumented test piles have been built on 60 by 50 m collection systems, each consisting of lysimeters and a large impermeable high-density polyethylene liner. Collection lysimeters are installed nearby to investigate infiltration in the upper 2 m of the waste rock. Porosity, water retention curves, and hydraulic conductivity functions are estimated from field measurements and for samples ranging in size from 200 cm^3 to 16 m^3. Net infiltration in 2007 is estimated to have been 37% of the rainfall for mean annual rainfall conditions. Early-season infiltration freezes and is remobilized as the waste rock thaws. Wetting fronts migrate at rates of 0.2–0.4 $m\,d^{-1}$ in response to common rainfall events and up to 5 $m\,d^{-1}$ in response to intense rainfall. Pore water and non-reactive solutes travel at rates of $<10^{-2}$ to 3×10^{-2} $m\,d^{-1}$ in response to common rainfall events and up to 0.7 $m\,d^{-1}$ in response to intense rainfall. Time-varying SO_4 mass loading from the base of the test piles is dictated primarily by the flow behaviour, rather than by changes in solute concentrations.

14/01748 The impact of human behavior on ecological threshold: positive or negative? – grey relational analysis of ecological footprint, energy consumption and environmental protection

Huimin, L. *Energy Policy*, 2013, 56, 711–719.

Human behaviour has the positive and negative impact on ecosystem. To study the interaction between ecosystem and behaviour system, per-capita energy ecological footprint (EEF) is selected as the ecosystem threshold. Elasticity coefficient of environmental investment (ECEI) and elasticity coefficient of energy consumption (ECEC) represent the positive and negative human impact on ecosystem, respectively. It takes Shanghai, China as the empirical area to implement grey relational analysis of per-capita EEF (consist of coal, coke, fuel oil and electricity), ECEC and ECEI from 1978 to 2010. The grey correlation coefficients show that negative behaviour of energy consumption has the closer influence on the ecosystem than positive behaviour of environmental protection. Electricity is the most significant factor of the energy consumption and the highest sensitive indicator to the environmental capital input–output. From the perspective of government policy, 'energy saving' is more efficient than 'emissions reduction'. Reducing the negative activities is imminent in the current process of development.

14/01749 The influence of meteorological factors and biomass burning on surface ozone concentrations at Tanah Rata, Malaysia

Toh, Y. Y. *et al*. *Atmospheric Environment*, 2013, 70, 435–446.

The surface ozone concentrations at the Tanah Rata regional Global Atmosphere Watch station, Malaysia (4°28′N, 101°23′E, 1545 m above Mean sea level) from June 2006 to August 2008 were analysed in this study. Overall the ozone mixing ratios are very low; the seasonal variations show the highest mixing ratios during the south-west monsoon (average 19.1 ppb) and lowest mixing ratios during the spring inter-monsoon (average 14.2 ppb). The diurnal variation of ozone is characterized by an afternoon maximum and night-time minimum. The meteorological conditions that favour the formation of high ozone levels at this site are low relative humidity, high temperature and minimum rainfall. The average ozone concentration is lower during

precipitation days compared to non-precipitation days. The hourly averaged ozone concentrations show significant correlations with temperature and relative humidity during the north-east monsoon and spring inter-monsoon. The highest concentrations are observed when the wind is blowing from the west. The authors found an anticorrelation between the atmospheric pressure tide and ozone concentrations. The ozone mixing ratios do not exceed the recommended Malaysia air quality guidelines for 1- and 8-h averages. Five-day backward trajectories on two high ozone episodes in 7 August 2006 (40.0 ppb) and 24 February 2008 (45.7 ppb) are computed using the hybrid single-particle Lagrangian integrated trajectory model to investigate the origin of the pollutants and influence of regional transport. The high ozone episode during 7 August 2006 (burning season during the south-west monsoon) is mainly attributed to regional transport from biomass burning in Sumatra, whereas favourable meteorological conditions (i.e. low relative humidity, high temperature and solar radiation, zero rainfall) and long-range transport from Indo-China have elevated the ozone concentrations during 24 February 2008.

14/01750 The use of electrochemical sensors for monitoring urban air quality in low-cost, high-density networks

Mead, M. I. *et al. Atmospheric Environment*, 2013, 70, 186–203.

Measurements at appropriate spatial and temporal scales are essential for understanding and monitoring spatially heterogeneous environments with complex and highly variable emission sources, such as in urban areas. However, the costs and complexity of conventional air quality measurement methods means that measurement networks are generally extremely sparse. This paper shows that miniature, low-cost electrochemical gas sensors, traditionally used for sensing at parts-per-million (ppm) mixing ratios can, when suitably configured and operated, be used for parts-per-billion (ppb) level studies for gases relevant to urban air quality. Sensor nodes, in this case consisting of multiple individual electrochemical sensors, can be low-cost and highly portable, thus allowing the deployment of scalable high-density air quality sensor networks at fine spatial and temporal scales, and in both static and mobile configurations. This paper provides evidence for the performance of electrochemical sensors at the parts-per-billion level, and then outlines the results obtained from deployments of networks of sensor nodes in both an autonomous, high-density, static network in the wider Cambridge (UK) area, and as mobile networks for quantification of personal exposure. Examples are presented of measurements obtained with both highly portable devices held by pedestrians and cyclists, and static devices attached to street furniture. The widely varying mixing ratios reported by this study confirm that the urban environment cannot be fully characterized using sparse, static networks, and that measurement networks with higher resolution (both spatially and temporally) are required to quantify air quality at the scales which are present in the urban environment. It is concluded that the instruments described here, and the low-cost/high-density measurement philosophy which underpins it, have the potential to provide a far more complete assessment of the high-granularity air quality structure generally observed in the urban environment, and could ultimately be used for quantification of human exposure as well as for monitoring and legislative purposes.

14/01751 'This is not a burning issue for me': how citizens justify their use of wood heaters in a city with a severe air pollution problem

Reeve, I. *et al. Energy Policy*, 2013, 57, 204–211.

Although wood smoke pollution has been linked to health problems, wood burning remains a popular form of domestic heating in many countries across the world. This study describes the rhetoric of resistance to wood heater regulation amongst citizens in the regional Australian town of Armidale, where wood smoke levels regularly exceed national health advisory limits. The authors discuss how this is related to particular sources of resistance, such as affective attachment to wood heating and socio-cultural norms. The research draws on six focus groups with participants from households with and without wood heating. With reference to practice theory, the authors argue that citizen discourses favouring wood burning draw upon a rich suite of justifications and present this activity as a natural and traditional activity promoting comfort and cohesion. Such discourses also emphasize the identity of the town as a rural community and the supposed *gemeinschaft* qualities of such places. It is shown that, in this domain of energy policy, it is not enough to present 'facts' which have little emotional association or meaning for the populace. Rather, there is a need to understand how social scripts, often localized, inform identity and practice.

14/01752 Wetlands are an effective green roof system

Song, U. *et al. Building and Environment*, 2013, 66, 141–147.

Green roofs recently have garnered much attention as a means to reduce both the absorption of solar energy in summer and heat loss in winter, especially in urban areas with limited space for gardening. Constructed wetland roofs maintain more stable temperature profiles than terrestrial systems because of their slow heat transfer and high heat storage capacity. The authors found that wetland roofs were particularly efficient at decreasing the temperature of green roof systems on hot days. Wetland plants have high evaporation rates that are associated with their ability to cool buildings. Constructed wetland had excellent water holding ability, requiring less than 400 l water/m^2 of irrigation over the entire growing season, which was less than 20% of the expected irrigation requirement for terrestrial systems on green rooftops. Wetland macrophyte species demonstrated high tolerance to flooding and drought and showed great potential for regeneration by rhizomes, suggesting easy maintenance. Plants grown in the constructed wetland accumulated high biomass that can serve as a carbon sink. Wetlands on rooftops would not exceed the weight-bearing capacity of rooftops if water depths are designed and kept under 30 cm. Constructed-wetland roofs offer thermal benefits, a low amount of required irrigation, high tolerance of drought and flood, and flood-control capacities. They also can act as a carbon sink, are easy to manage, and provide other ecological services. Therefore, constructed wetlands are a reasonable choice for green rooftop systems.

CO_2, NO_x, SO_2 and particulate emissions

14/01753 Adsorption of SO_x by oxide materials: a review

Mathieu, Y. *et al. Fuel Processing Technology*, 2013, 114, 81–100.

This paper is an attempt to provide a review of the literature devoted to the wide variety of sorbent systems that are currently either in use or under laboratory investigation for the removal of the SO_x ($SO_2 + SO_3$) from flue gases. From an industrial perspective and besides any economic consideration, 'the ideal' SO_x sorbent candidate must ally four essential qualities some of which may appear contradictory to some extent: a strong affinity of the sorbent towards SO_x along with fast kinetics; a large specific surface; a high physical/thermal/chemical stability and the capability for multiple regenerations at a reasonable temperature and with performance recoveries close to 100%. In this paper, the sorbent are classified in four categories which are: (i) single oxides; (ii) mixed oxides (including spinels and alumina supported oxides); (iii) oxides supported on carbonaceous materials and (iv) oxides supported on zeolites and mesoporous materials. A noteworthy outcome of this review lies in the promising prospects offered by porous silica-based materials as desulfurization ('DeSOx') candidates and the interest of elaborating in this direction.

14/01754 Analysis and control design of sustainable policies for greenhouse gas emissions

Chu, B. *et al. Applied Thermal Engineering*, 2013, 53, (2), 420–431.

Reducing greenhouse gas emissions is now an urgent priority. Systems control theory, and in particular feedback control, can be helpful in designing policies that achieve sustainable levels of emissions of CO_2 (and other greenhouse gases) while minimizing the impact on the economy, and at the same time explicitly addressing the high levels of uncertainty associated with predictions of future emissions. This paper describes the preliminary results for an approach where model predictive control (MPC) is applied to a model of the UK economy (UK 4see model) as a test bed to design sustainable policies for greenhouse gas emissions. Using feedback control, the policies are updated on the basis of the actual emissions, rather than on the predicted level of emissions. The basic structure and principle of the UK 4see model is described and its implementation in Simulink is presented. A linearized state space model is obtained and model predictive control is applied to design policies for CO_2 emissions. Simulation results are presented to demonstrate the effectiveness of the proposed method. The preliminary results obtained in this paper illustrate the strength of the proposed design approach and form the basis for future research on using systems control theory to design optimal sustainable policies.

14/01755 Analyzing the driving forces behind CO_2 emissions and reduction strategies for energy-intensive sectors in Taiwan, 1996–2006

Huang, Y.-H. and Wu, J.-H. *Energy*, 2013, 57, 402–411.

Between 1996 and 2006, CO_2 emissions in Taiwan increased by approximately 60%, with the industrial sector accounting for 50% of that increase. Among all industrial sectors, iron and steel, petrochemicals, electronics, textiles, pulp and paper and cement accounted for approximately three-quarters of the total industrial CO_2 emissions. Identifying the driving forces behind increased CO_2 emissions in these six sectors could be valuable for the development of effective environmental policy. This study used two-tier KLEM input–output structural decomposition analysis (I-O SDA) to analyse the factors that

lead to changes in CO_2 emissions. Empirical results obtained in Taiwan reveal that increased exports level and elevated domestic autonomous final demand level were the main reasons for increases in CO_2 emissions. Technological changes in materials and labour tended to decrease CO_2 emissions, while the power generation mix contributed significantly to the increase. Relevant strategies for reducing CO_2 emissions from energy-intensive sectors are also highlighted.

14/01756 Characteristics of an advanced carbon sorbent for CO_2 capture

Hornbostel, M. D. *et al. Carbon*, 2013, 56, 77–85.

The adsorption and desorption characteristics on an advanced carbon sorbent for gases present in the flue gas stream, including CO_2, N_2, O_2, Ar, H_2O vapour, and impurities NO and SO_2 are discussed. At 5 °C and 1 atm CO_2 pressure, this carbon sorbent can uptake 20 wt% (or 4.5 mmol/g) of CO_2, with high Henry's law selectivity over N_2, O_2 and Ar. The heat of adsorption for CO_2 decreases from ~28 kJ/mol (290 meV) to ~25.7 kJ/mol (260 meV) as the coverage of CO_2 increases; whereas the heat of adsorption for N_2, O_2 and Ar is in the range of 16–17 kJ/mol. The carbon sorbent has a high surface area of 1270 m^2/g, high thermal conductivity (0.8 W/m K), low heat capacity (1 J/g K), high mechanical strength, and high attrition resistance. It is an ideal candidate for post-combustion CO_2 capture using rapid pressure swing and rapid temperature swing methods.

14/01757 CO_2 fixation for succinic acid production by engineered *Escherichia coli* co-expressing pyruvate carboxylase and nicotinic acid phosphoribosyltransferase

Liu, R. *et al. Biochemical Engineering Journal*, 2013, 79, 77–83.

In wild-type *Escherichia coli*, 1 mol of CO_2 was fixated in 1 mol of succinic acid generation anaerobically. The key reaction in this sequence, catalysed by phosphoenolpyruvate carboxylase (PPC), is carboxylation of phosphoenolpyruvate to oxaloacetate. Although inactivation of pyruvate formate-lyase and lactate dehydrogenase is found to enhance the PPC pathway for succinic acid production, it results in excessive pyruvic acid accumulation and limits regeneration of NAD^+ from NADH formed in glycolysis. In other organisms, oxaloacetate is synthesized by carboxylation of pyruvic acid by pyruvate carboxylase (PYC) during glucose metabolism, and in *E. coli*, nicotinic acid phosphoribosyltransferase (NAPRTase) is a rate-limiting enzyme of the NAD(H) synthesis system. To achieve the $NADH/NAD^+$ ratio decrease as well as carbon flux redistribution, co-expression of NAPRTase and PYC in a *pflB*, *ldhA*, and *ppc* deletion strain resulted in a significant increase in cell mass and succinic acid production under anaerobic conditions. After 72 h, 14.5 g L^{-1} of glucose was consumed to generate 12.08 g L^{-1} of succinic acid. Furthermore, under optimized condition of CO_2 supply, the succinic acid productivity and the CO_2 fixation rate reached 223.88 and 83.48 mg L^{-1} h^{-1}, respectively.

14/01758 Determination of the inter-annual and spatial characteristics of the contribution of long-range transport to SO_2 levels in Seoul between 2001 and 2010 based on conditional potential source contribution function (CPSCF)

Jeong, U. *et al. Atmospheric Environment*, 2013, 70, 307–317.

This paper introduces a new method to estimate the change in mean mixing ratio of a target species at a receptor site due to the contribution of the long-range transport (CLRT). The authors applied this method to determine inter-annual and inter-seasonal variations in the CLRT of SO_2 in Seoul, a major megacity in north-eastern Asia, during the period from 2001 to 2010. The major potential source areas of SO_2 for the 2001–2010 period were located in east China according to the potential source contribution function maps. The CLRT of SO_2 in Seoul was estimated to range from 0.40 to 1.03 ppb, which accounted for 8–21% of the ambient mean SO_2 mixing ratio in Seoul. The inter-annual variations of estimated CLRT of SO_2 was well correlated with those of the total emissions in China during the period from 2001 to 2008 ($R = 0.85$). It was found that both local emissions from around Seoul and long-range transport from east China, especially the Shandong peninsula, affected the SO_2 mixing ratio in Seoul throughout the decade of study. The CLRT of SO_2 in Seoul increased after 2007 even though the total emissions of SO_2 by China have been decreasing since 2006. The CLRT of SO_2 in Seoul was high in spring and winter, which can be attributed to enhanced SO_2 emissions in east China during these seasons and a dominant westerly wind. The CLRTs of SO_2 accounted for 15, 11, 4 and 12% of the seasonal mean SO_2 mixing ratio in spring, summer, autumn and winter, respectively. The uncertainty ranged from 24 to 62% of the estimated CLRT values.

14/01759 Enhancement of attrition resistance and cyclic CO_2 capture of calcium-based sorbent pellets

Chen, H. *et al. Fuel Processing Technology*, 2013, 116, 116–122.

Calcination/carbonation of calcium-based sorbent is considered one of the most promising technologies to capture CO_2. The attrition resistance and CO_2 uptake of Ca-based sorbent were of great concern. Efforts were made to enhance the attrition resistance of sorbents primarily by making sorbent pellets with aluminate cements and maintain high CO_2 capture capacity of sorbents by adding pore forming agents. Batch experiments were conducted in a fluidized bed to investigate the effect of parameters on sorbent attrition. CO_2 capture performance of the pellets was also examined in a calcination/carbonation reactor system. The pore structure characteristics (BET, BJH) were measured as a supplement to the attrition and reaction studies. Results showed that the mechanical property of the pellets with 10 wt% aluminate cement was greatly enhanced. While, CO_2 capture capacity of the pellets made with 10 wt% aluminate cement and 5–10 wt% pores forming agent was greatly increased and displayed much slower decay during multiple cycles compared with the original limestone. This was attributed to the large number of mesopores caused by the use of chemical agents and the exposure of inner core of CaO sorbents due to the attrition, which are in favour of CO_2 capture. The pore structure showed that the BET surface area and BJH pore volume were expanded by adding pore forming agents, which benefits CO_2 uptake of the sorbents during the cycling.

14/01760 Enhancement of dissolved inorganic carbon and carbon fixation by green alga *Scenedesmus* sp. in the presence of alkanolamine CO_2 absorbents

Kim, G. *et al. Biochemical Engineering Journal*, 2013, 78, 18–23.

The influence of alkanolamine CO_2 absorbents on the CO_2 fixation in photoautotrophic culture of green alga *Scenedesmus* sp. was investigated using monoethanolamine (MEA), 2-amino-2-methyl-1-propanol (AMP), diethanolamine (DEA) and triethanolamine (TEA). The dissolved inorganic carbon (DIC) contents increased when alkanolamine compounds existed in the medium. Utilizing the increased DIC for algal uptake, TEA exhibited a best enhancement in CO_2 fixation performance compared to other absorbents, while primary ethanolamines displayed inhibition on cell growth due to the formation of relatively stable carbamate intermediate. By adding 5 mM TEA, the cell growth and CO_2 fixation rate increased by 30.5% compared to the case with no TEA. TEA was supplemented when cell density was doubled, tripled and quadrupled to maintain the TEA to cells ratio constant pacing the increase of cell density. The repeated addition of TEA exhibited the enhancement of CO_2 fixation rate by 39.3% and 18.5% from no-addition and one-time addition cases, respectively.

14/01761 Experimental performance evaluation for a carbon dioxide light commercial cooling application under transcritical and subcritical conditions

Boccardi, G. *et al. Applied Thermal Engineering*, 2013, 54, (2), 528–535.

In this paper the results of an experimental investigation on a small capacity, air-forced refrigerating plant working with CO_2 are presented. The air inlet temperatures at gas cooler and evaporator were varied between 16 and 31 °C and between −25 and +25 °C, respectively, to cover the range of temperatures under conditions typical of commercial refrigeration, during quasi-steady operation. The thermodynamic analysis of the system performance was carried on varying independently the pressure at the gas cooler, by overfeeding the liquid receiver to point out the effect of refrigerant charge. The results allow to describe the performance of the system in a map varying the boundary conditions; at the same time the corresponding variations of the thermodynamic cycle, the coefficient of performance and the mass flow rate are reported.

14/01762 Facultative autotrophic denitrifiers in denitrifying sulfide removal granules

Lee, D.-J. *et al. Bioresource Technology*, 2013, 132, 356–360.

The denitrifying sulfide removal (DSR) process applied autotrophic and heterotrophic denitrification pathways to achieve simultaneous conversion of nitrate to N_2, sulfide to elementary sulfur, and organic substances to CO_2. However, autotrophic denitrifiers and heterotrophic denitrifiers have to grow at comparable rates so the long-term DSR stability can be maintained. This work assessed the autotrophic and heterotrophic denitrification activities by 16 isolates from anaerobic granules collected from a DSR-expanded granular sludge bed reactor. A group of strains with closest relatives as *Pseudomonas* sp. (89.9–98.3% similarity), *Agrobacterium* sp. (94.6% similarity) and *Acinetobacter* sp. (96.6% similarity) were identified with both autotrophic and heterotrophic denitrification capabilities. These facultative autotrophic denitrifiers can be applied as potential strains for lifting the limitation by balanced growth of two distinct bacterial groups in the DSR reactor.

14/01763 Household carbon dioxide emissions from peasants and herdsmen in northwestern arid-alpine regions, China

Qu, J. *et al. Energy Policy*, 2013, 57, 133–140.

This study assessed CO_2 emissions (related to the consumption of necessary and luxury goods and services) of the households of peasants and herdsmen in arid-alpine regions in Gansu, Qinghai and Ningxia provinces, China. The authors also explored whether agriculture types,

family income and family size have played any role in household CO_2 emissions. In order to address these issues: (i) assessment indicators for household emissions were developed; (ii) semi-structured questionnaire household surveys were conducted and (iii) input–output analysis (IOA) was employed. The results showed that, the average household CO_2 emission per capita is 1.43 tons (t) CO_2; the proportion of subsistence emissions (related to the consumption of necessary goods and services) accounts for 93.24%, whereas luxury emissions (generated due to consumption of specific goods and services that are consumed only when household income improves) only account for 6.76%t. Moreover, household CO_2 emissions increase with family income and family size, but per capita emissions are inversely related to family size. The highest average household emissions were found in the alpine agricultural and pastoral region (6.18 t CO_2), followed by the irrigated agricultural region (6.07 t CO_2) and the rain-fed agricultural region (5.34 t CO_2). In consideration of insignificant amount of household emissions from these poor and vulnerable groups of the society, this study suggests to follow the principle of fairness while making energy conservation, emission reduction and adaptation policies.

14/01764 In situ synthesis of CuSAPO-34/cordierite and its selective catalytic reduction of nitrogen oxides in vehicle exhaust: the effect of HF

Wang, J. *et al. Fuel*, 2013, 109, 101–109.

CuSAPO-34/cordierite catalysts were prepared via *in situ* hydrothermal synthesis technique with and without HF. The morphology and structure of the synthesized samples were characterized in the present work. The NO_x selective catalytic reduction (SCR) activities of the catalysts were evaluated with a fixed-bed reactor in simulated diesel vehicle exhaust. The results indicate that the addition of HF into the initial gel during the preparation of CuSAPO-34/cordierite can accelerate the crystallization and improve the relative crystallinity of CuSAPO-34, which lead to the compact morphology of the products. Furthermore, the existence of HF can increase the specific pore volume, BET surface area and CuSAPO-34 loading of the catalyst. For the crystallization time of 24 h, the loading amounts of CuSAPO-34 are 20.3 and 13.6 wt% for the samples prepared with and without HF, respectively. The obvious improvement of the catalytic activities for NO_x removal has been obtained over the catalysts prepared with HF. The active temperature window (NO_x conversion rate > 95%) of the samples prepared with HF is wider (340–600 °C) than the samples prepared without HF (440–540 °C). The catalysts with HF present great endurance ability for the aging treatment at 650 °C with 15 vol.% H_2O. The low temperature activity for NO_x removal of the catalyst prepared with HF is not affected by the aging treatment and the maximum NO_x conversion rate of the aging catalyst at the crystallization time of 12 h is about 96%, but only 80% for the catalyst without HF. The roles of HF and the different performances of the samples prepared with and without HF were discussed with the aid of X-ray powder diffraction, scanning electron microscopy and X-ray photoelectron spectroscopy techniques.

14/01765 Indoor–outdoor relationships of airborne particles and nitrogen dioxide inside Parisian buses

Molle, R. *et al. Atmospheric Environment*, 2013, 69, 240–248.

This study evaluated passengers' exposure to traffic air pollution inside the articulated buses of the line 91 in Paris during 10 working days in May 2010. Twenty articulated buses were studied on 32 routes in order to determine the influence of the sampling position on the pollutant concentrations. This parameter is still poorly known for the rigid buses and is even less known for the articulated ones. However this parameter must be studied for articulated buses because the greater length may cause a pollutant concentration gradient in the cabin. Portable devices were used to measure pollutants in the presence of passengers from 8 to 9 am and from 4 to 5 pm, time periods corresponding to the peak traffic and travellers. $PM_{2.5}$ mass concentration, particle number concentration between 0.3 and 20 μm and nitrogen dioxide concentration were simultaneously measured on three positions inside the buses (front, middle and rear) in order to study the spatial distribution of these compounds. These measurements inside the buses were compared to the outdoor concentrations at the same moment of the day provided by the Parisian air quality monitoring network; they were also compared to the results of a previous monitoring campaign performed in 2008. The results obtained during the 2010 campaign revealed that in-cabin NO_2 mean concentrations were 1.5–3.5 times higher than the outside concentration levels; a maximum concentration of $234 \pm 40\,\mu g\,m^{-3}$ was found in the rear position (location of the engine and exhaust gas). Mean in-cabin $PM_{2.5}$ mass concentrations varied from one week to another, but they were globally the same at the three positions inside the instrumented buses. In order to determine the impact of outdoor levels, correlations have been calculated between the results measured inside the buses and those measured by the outdoor air monitoring stations. The highest Pearson correlation coefficient was 0.29 for NO_2 data whereas the highest Pearson correlation coefficient between in-cabin $PM_{2.5}$ mass concentrations and outdoor levels was 0.96. The higher indoor/outdoor correlation of $PM_{2.5}$ compared to NO_2 may result from the high variation of $PM_{2.5}$ outdoors. Otherwise, this low indoor/outdoor correlation of NO_2 can highlight a source of pollution other than the outdoor air.

14/01766 Metal-doped carbon xerogels for the electro-catalytic conversion of CO_2 to hydrocarbons

Pérez-Cadenas, A. F. *et al. Carbon*, 2013, 56, 324–331.

Original carbon xerogels doped with transition metals Ni, Cu or Fe have been prepared as cathodes for the electro-catalytic reduction of CO_2 at atmospheric pressure. Commercial metallic and carbon materials have been also tested as cathodes for comparison, and the leaching of Ni-based cathodes during reaction has been analysed. Carbon xerogels doped with transition metals work very well as electro-catalysts in the transformation of CO_2 to gaseous hydrocarbons C_1–C_4. The product distribution strongly depends on the metal. In this reduction process not only the type of metal but also the textural and chemical properties of the carbon xerogel play an important role in the electro-catalytic performance. The use of xerogel-based electrodes considerably reduces the amount of transition metal required.

14/01767 Modeling CO_2–brine–rock interactions in the Knox Group: implications of a deep carbon storage field test in western Kentucky

Zhu, J. *et al. Applied Geochemistry*, 2013, 37, 29–42.

The Cambrian–Ordovician Knox Group, a thick sequence of dolostone and minor dolomitic sandstone, is a prospective CO_2 sequestration target in the southern Illinois Basin, USA. Thorough evaluation of the Knox Group is critical because the main sequestration target elsewhere in the Illinois Basin, the Cambrian Mount Simon Sandstone, is thin or absent throughout most of Kentucky. A 2477-m-deep carbon storage test well in Hancock County, Kentucky, was drilled, and 626 metric tons of CO_2 was injected into the Knox saline reservoirs. To understand the long-term fate of CO_2 injected into the Knox reservoirs, geochemical reactions between CO_2, brine and rock-forming minerals were modelled using TOUGHREACT. The modelling benefited from a robust data set collected from the test well, including core porosity and permeability, petrographic and X-ray powder diffraction mineralogy, brine chemistry, temperature and pressure measurements. Kinetic batch models and two-dimensional (2-D) radial reactive transport models were used to evaluate the migration of the injected CO_2, changes in brine chemistry, and mineral dissolution and precipitation. Results from the kinetic models suggest that sections of the Knox dominated by dolomite have very limited mineral-trapping capacity for CO_2, whereas thin sections of dolomitic sandstone with aluminosilicate minerals such as K-feldspar facilitate mineral trapping. The 2-D model for the CO_2 injection test suggests that, because of the presence of thick permeable intervals in the Knox and the small volume of injected CO_2 in the test, the radius of influence is less than 11 m from the well. The hypothetical long-term injection model indicates, on the other hand, that commercial-scale injection would influence a much larger area and part of the injected CO_2 remains in the supercritical/gas phase for a long time. Because of the buoyancy effect, most supercritical/gas-phase CO_2 migrates upward and stays in the top of the reservoirs dominated by dolomite with small mineral-trapping capacity.

14/01768 NO_x emission characteristics of superfine pulverized anthracite coal in air-staged combustion

Shen, J. *et al. Energy Conversion and Management*, 2013, 74, 454–461.

Superfine pulverized coal combustion is a new pulverized coal combustion technology that has better combustion stability, higher combustion efficiency, and comprehensive cost-effective operation. In this paper, the experiment of YQ anthracite coal combustion was carried out on an electrically heated drop tube furnace. Meanwhile, single air staged and multi air staged combustion were both adopted to understand NO_x emission behaviours and analysis of mechanism and reaction pathways of each experimental phenomenon was proposed as well. The results indicate that the NO_x reduction efficiency of superfine pulverized coal (22.5–32%) in single staged combustion is higher than that of regular particle size (10%). The NO_x abatement in multi-air-staged combustion is greater than that in single-air-staged combustion. In multi-air-staged combustion, the NO_x reduction efficiency of superfine pulverized coal is superior to that of regular size, which may be due to the reaction mechanism where further penetration and adsorption of NO_x takes place in the inner pores. Particle burnout in multi-staged combustion ratio was found to be irrelevant to the operating conditions. The findings of this paper will provide useful data for the subsequent experiment to investigate into the mechanism of pure NO–char reduction and for the basis of W-flame furnace operation.

14/01769 NO_x emissions from a central California dairy

Hasson, A. S. *et al. Atmospheric Environment*, 2013, 70, 328–336.

Concentrations of NO_x ($NO + NO_2$) were monitored downwind from a dairy facility in central California, USA, during 2011 and 2012. NO_x concentrations at the dairy were significantly higher than the background levels during August 2011 primarily due to the presence of elevated NO, but were indistinguishable from background concentrations during January and April 2012. A Gaussian plume model (AERMOD) and a Lagrangian back trajectory model (Wind Trax) were used to estimate the flux of NO from the dairy during August 2011 with the assumption that emissions were primarily from animal feed. NO emissions from silage were also directly measured from feed to provide additional insight into the sources. Isolation flux chamber measurements imply an NO flux from the feed of about $1.3 \times 10^{-3}\,g\,m^{-2}\,h^{-1}$, but these relatively low fluxes are inconsistent with the elevated NO concentrations observed during August 2011. This implies that either the flux chamber method grossly underestimates the true NO emissions from feed, or that most of the ambient NO measured at the dairy is from other sources. Emissions from farm machinery may account for the NO concentrations observed. Animal feed thus appears to be a small contributor to NO_x emissions within central California.

14/01770 Particulate emissions from the co-combustion of forest biomass and sewage sludge in a bubbling fluidised bed reactor

Calvo, A. I. *et al. Fuel Processing Technology*, 2013, 114, 58–68.

In the present study, particulate emissions from the co-combustion of forest biomass residues with sewage sludge in a pilot-scale bubbling fluidized bed combustor were characterized. The combustion flue gas was exhausted to the atmosphere after passing through a cyclone separator. Physical–chemical characteristics of the particles were studied: (i) morphology and aerosol size, surface and volume distributions before the cyclone and (ii) chemical composition (carbonates, water soluble-inorganic ions, organic and elemental carbon) before and after the cyclone. Chemical composition data were used to calculate aerosol density and refractive index. Aerosols showed a unimodal size distribution with a geometric mean diameter of $2.25 \pm 0.02\,\mu m$ and a geometric standard deviation of 1.27 ± 0.01. The surface and volume mean diameters were 2.64 ± 0.02 and $2.91 \pm 0.05\,\mu m$, respectively. Water-soluble inorganic ions were predominant in the fine particle fraction ($PM_{2.5}$). The filters were loaded of crystallized mineral particles. The analysis revealed a dominance of calcium carbonate/oxide and halide (NaCl or KCl), sulfate and aluminosilicate nanocrystals forming larger mixed aggregates.

14/01771 Particulate matter concentrations, physical characteristics and elemental composition in the Milan underground transport system

Colombi, C. *et al. Atmospheric Environment*, 2013, 70, 166–178.

An extensive measurement campaign was conducted in the Milan subway system in order to investigate PM10 concentrations, to determine its physical and elemental composition, its origins, and to attempt to quantify source contributions. The Milan subway system includes three lines and stations typically consist of two underground levels: an intermediate floor (mezzanine) where the turnstiles for accessing the platform are located, and a platform level, one floor down. Measurements were performed in two stations for each line, and both microenvironments (platform and mezzanine) were investigated in all cases. PM10 samples were collected at all twelve sites over three daily periods for nine consecutive days at each site. Particle number concentrations were also measured with optical particle counters and size-number distributions were determined. X-ray fluorescence analysis was also performed on the samples to determine element concentrations. The results indicate PM sources related with train operations as the dominant impact on particulate concentrations. Average weekday PM10 concentrations between 105 and $283\,\mu g\,m^{-3}$ were observed at the platform level, while average ambient concentrations of $36\,\mu g\,m^{-3}$ were observed. Fe, Ba, Sb, Mn and Cu were found to be significantly enriched. Metal particles, occurring mostly in the range of diameters between 1 and $5\,\mu m$, and therefore likely originating from mechanical processes, account for most of the PM10 mass at the platform level. Wheel, brake and track wear are found to contribute 40–73% of total PM10 mass and electric cable wear (Cu and Zn oxides) 2–3%. Concentrations measured on the mezzanine levels are intermediate between those found in ambient air and on the platform level, with average daytime PM10 values ranging from 50 to $80\,\mu g\,m^{-3}$. The situation observed on the mezzanine can well be described through an appropriate mixing of ambient and platform level air. A decreasing, albeit still significant, impact from internal sources is observed, with particulate from wheel, brake and track wear contributing an average of 2–25%, and electric cable wear 0.5–1.2%, to total PM10 mass.

14/01772 Prediction of CO_2 loading capacity of chemical absorbents using a multi-layer perceptron neural network

Bastani, D. *et al. Fluid Phase Equilibria*, 2013, 354, 6–11.

A feed forward multi-layer perceptron neural network was developed to predict carbon dioxide loading capacity of chemical absorbents over wide ranges of temperature, pressure, and concentration based on the molecular weight of solution. To verify the suggested artificial neural network (ANN), regression analysis was conducted on the estimated and experimental values of CO_2 solubility in various aqueous solutions. Furthermore, a comparison was performed between results of the proposed neural network and experimental data that were not previously used for network training, as well as a set of data for binary solutions. Comparison between the proposed multi-layer perceptron (MLP) network and other alternative models illustrated some notable points: (1) better performance of the proposed model, (2) extrapolation capabilities of the network, (3) unlimited ranges of network performance regardless of parameters such as temperature, pressure, and concentration and (4) ability of using MLP network as a correlation for prediction of carbon dioxide loading for different aqueous solutions.

14/01773 Reconciling NO_x emissions reductions and ozone trends in the U.S., 2002–2006

Zhou, W. *et al. Atmospheric Environment*, 2013, 70, 236–244.

Dynamic evaluation seeks to assess the ability of photochemical models to replicate changes in air quality as emissions and other conditions change. When a model fails to replicate an observed change, a key challenge is to discern whether the discrepancy is caused by errors in meteorological simulations, errors in emission magnitudes and changes, or inaccurate responses of simulated pollutant concentrations to emission changes. In this study, the community multiscale air quality (CMAQ) model is applied to simulate the ozone (O_3) change after the NO_x SIP Call and mobile emission controls substantially reduced nitrogen oxides (NO_x) emissions in the eastern USA from 2002 to 2006. For both modelled and observed O_3, changes in episode average daily maximal 8-h O_3 were highly correlated ($R^2 = 0.89$) with changes in the 95th percentile, although the magnitudes of reductions increased non-linearly at high percentile O_3 concentrations. Observed downward changes in mean NO_x (-11.6 to -2.5 ppb) and 8-h O_3 (-10.4 to -4.7 ppb) concentrations in metropolitan areas in the NO_x SIP Call region were under-predicted by 31%–64% and 26%–66%, respectively. The under-predicted O_3 improvements in the NO_x SIP Call region could not be explained by adjusting for temperature biases in the meteorological input, or by considering uncertainties in the chemical reaction rate constants. However, the under-prediction in O_3 improvements could be alleviated by 5%–31% by constraining NO_x emissions in each year based on observed NO_x concentrations. This demonstrates the crucial need to accurately characterize changes in precursor emissions when dynamically evaluating a model's ability to simulate O_3 responses to those changes.

14/01774 Sn-modified NO_x storage/reduction catalysts

Pieta, I. S. *et al. Catalysis Today*, 2013, 207, 200–211.

Ba-, K-, and Ba–K-based NO_x storage/reduction (NSR) catalysts were prepared, with and without Sn as a promotor. Catalysts and catalyst/soot mixtures were evaluated for NO_x reduction and soot oxidation under standard NSR cycling conditions. The activity study was accompanied by dispersion measurements, TEM, XRD, and XPS characterization. It was found that modification with Sn did not significantly influence NO_x adsorption, however, Sn notably enhanced soot oxidation for Ba-based systems. This was correlated to Pt oxidation state modification. Also the addition of Sn to the Pt–Ba and Pt–Ba–K catalysts lowered the onset temperature of S release. The Pt–Ba–K catalyst had higher stability against S-poisoning, likely due to the preferential adsorption of S onto K-species, partially maintaining Ba sites for NO_x trapping.

14/01775 SO_2 adsorption products on Pt nanoparticles as a function of electrode potential and oxidative properties of carrier gas: in situ sulfur K-edge XANES approach

Baturina, O. A. *et al. Catalysis Today*, 2013, 205, 106–110.

In situ sulfur K-edge X-ray absorption near-edge structure spectroscopy is used to determine the nature of adsorbed SO_2 species from a SO_2/O_2 gas mixture on carbon-supported Pt nanoparticles (Pt/VC). SO_2 was adsorbed onto electrodes held at 0.1, 0.5, 0.7 and 0.9 V vs a reversible hydrogen electrode while flowing 1000 ppm SO_2 in O_2 through the working electrode compartment. SO_2 adsorption products from SO_2/O_2 are compared to those from SO_2/N_2 gas mixtures. The SO_2 adsorption products are found to be essentially the same at electrodes held at 0.5, 0.7 and 0.9 V. A major difference is observed at 0.1 V, where (bi)sulfate ions are generated in the presence of SO_2 in O_2 likely due to a reaction between SO_2 and H_2O_2 formed as a byproduct of the oxygen reduction reaction in the hydrogen adsorption region. (Bi)sulfate generation on Pt/VC catalysts held at 0.1 V suggests that SO_2 may act as a peroxide radical scavenger at the proton exchange membrane fuel cell cathode. Although impurities such as SO_2 and H_2S usually promote hydrogen peroxide generation at the fuel cell cathodes, their detrimental effect may be diminished by their reaction with H_2O_2.

14/01776 The limited effect of EU emissions trading on corporate climate strategies: comparison of a Swedish and a Norwegian pulp and paper company
Gulbrandsen, L. H. and Stenqvist, C. *Energy Policy*, 2013, 56, 516–525.
This paper examines to what extent and how the European Union's emissions trading scheme (EU ETS) has influenced the climate strategies of two Nordic pulp and paper companies: Swedish SCA and Norwegian Norske Skog. Rising electricity prices are perceived to be the greatest effect of the scheme. The EU ETS has served to reinforce commitments to improve energy efficiency and reduce CO_2 emissions in both companies studied. Procedures like monitoring of CO_2 emissions and accounting for CO_2 prices have become more significant since the introduction of the EU ETS, but the scheme has not triggered a search for innovative, low-carbon solutions. Due to differences in market factors and production factors, SCA has been more active than Norske Skog in investing in and implementing CO_2-lean actions. Future studies of climate-mitigation activities, strategies and innovations in the pulp and paper industry should involve more in-depth investigation of the interactions between such factors and the EU ETS.

14/01777 Theoretical and experimental investigation of diesel engine with steam injection system on performance and emission parameters
Kökkülünk, G. *et al. Applied Thermal Engineering*, 2013, 54, (1), 161–170.
In this study, a new electronically controlled steam injection method is applied to a direct injection (DI) diesel engine to control NO_x emissions. This method can be also used to improve the performance and efficiency. Steam injected diesel engine is modelled by using zero-dimensional single-zone combustion model for 20% steam ratio at full load condition. The obtained results are compared with conventional diesel engine in terms of performance and NO, CO, CO_2, HC emissions. The simulation results agree with experimental data quite well. In the experimental results, it is determined that the engine torque and the effective power increase up to 2.5% at 1200 rpm, specific fuel consumption (SFC) and effective efficiency improves up to 6.1% at 2400 rpm, NO emissions reduce up to 22.4% at 1200 rpm, CO_2 emissions decrease up to 4.3% at 1800 rpm, smoke density increases from 44% to 46% at 2200 rpm. This paper may be a leading essential tool for the real-engine designers by considering the effects of steam injection into the engine cylinder.

14/01778 Trends in road freight transportation carbon dioxide emissions and policies in China
Li, H. *et al. Energy Policy*, 2013, 57, 99–106.
The authors adopted the simple average Divisia index approach to explore the impacts of factors on the carbon dioxide (CO_2) emissions from road freight transportation in China from 1985 to 2007. CO_2 emissions were investigated using the following as influencing factors: the emission coefficient, vehicle fuel intensity, working vehicle stock per freight transport operator, market concentration level, freight transportation distance, market share of road freight transportation, ton-kilometre per value added of industry, industrialization level and economic growth. Building on the results, the authors suggest that economic growth is the most important factor in increasing CO_2 emissions, whereas the ton-kilometre per value added of industry and the market concentration level contribute significantly to decreasing CO_2 emissions. They also discuss some recent important policies concerning factors contained in the decomposition model.

14/01779 Ultrafine particle concentrations in and around idling school buses
Zhang, Q. *et al. Atmospheric Environment*, 2013, 69, 65–75.
Unnecessary school bus idling increases children's exposure to diesel exhaust, but to what extent children are exposed to ultrafine particles (UFPs, with a diameter < 100 nm) in and around idling school buses remains unclear. This study employed nine school buses and simulated five scenarios by varying emissions source, wind direction, and window position. The purpose was to investigate the impact of idling on UFP number concentration and $PM_{2.5}$ mass concentration inside and near school buses. Near the school buses, total particle number concentration increased sharply from engine off to engine on under all scenarios, by a factor of up to 26. The impact of idling on UFP number concentration inside the school buses depended on wind direction and window position: wind direction was important and statistically significant while the effect of window positions depended on wind direction. Under certain scenarios, idling increased in-cabin total particle number concentrations by a factor of up to 5.8, with the significant increase occurring in the size range of 10–30 nm. No significant change of in-cabin $PM_{2.5}$ mass concentration was observed due to idling, regardless of wind direction and window position, indicating that $PM_{2.5}$ is not a good indicator for primary diesel exhaust particle exposure. The deposition rates based on total particle number concentration inside school bus cabins varied between 1.5 and 5.0 h^{-1} across nine tested buses under natural convection conditions, lower than those of passenger cars but higher than those of indoor environments.

14/01780 Using dual isotopes to evaluate sources and transformation of nitrogen in the Liao River, northeast China
Yue, F.-J. *et al. Applied Geochemistry*, 2013, 36, 1–9.
The Liao River Basin is one of seven primary river Basins in China. The concentration of dissolved inorganic nitrogen (DIN), dual isotopes of NO_3^- using the denitrifier method, the nitrogen isotopes of NH_4^+ and the nitrogen flux in the basin were determined to identify the sources of nitrogen and their transformation. The results show that NO_3^- ranges from 0.3 to 1316 μmol/L. In general, NO_3^- is the dominant inorganic nitrogen species during both flow seasons, but the fraction of NO_3^-/DIN is variable and high NH_4^+ is present in some waters. Samples collected from the up-stream portion of the Liao River typically had nitrogen isotope values of $<+8$‰, while those from the middle and lower portions had values of $>+8$‰ during the high flow season. Most water samples had oxygen isotope values of $<+10$‰ during the high flow season. During the low flow season, the ranges of nitrogen and oxygen isotopic values were limited, with average values of +10.3‰ and +4.9‰, respectively. There is a wider isotopic range of NO_3^- during the high flow season than the low flow season. The isotopic pattern of NO_3^- suggests that wastewater and soil organic nitrogen are the sources of NO_4^+ during the high flow season, while wastewater is the main source during low flow season. It appears that no intense denitrification occurs in the river according to the isotopic and chemical data. The nitrogen flux of the Liao River system entering the Liao Dong Bay annually is nearly 7.0×10^4 tons, which amounts to 5.0% of the nitrogen from chemical fertilizers used in this basin.

Hydrocarbon emissions

14/01781 Estimate of methane release from temperate natural wetlands using ENVISAT/SCIAMACHY data in China
Zhang, X. *et al. Atmospheric Environment*, 2013, 69, 191–197.
Since wetlands are the largest natural sources of atmospheric CH_4, it is important to estimate the CH_4 emissions from natural wetlands at regional scale and over a long time period. The annual CH_4 efflux from temperate natural wetlands excluding water surface in China was estimated, based on atmospheric CH_4 concentrations from SCIAMACHY/ENVISAT. The atmospheric CH_4 concentrations showed obvious seasonal cycles, and CH_4 emission from natural wetlands dominated the temporal variations of CH_4 concentrations in north China, accounting for about 67.94% of the variations of CH_4 concentrations. The chemical transport model, MOZART-4 (Model for Ozone and Related Chemical Tracers, version 4), was used to simulate the space-borne CH_4 column concentrations to the surface level, and then the relationship between surface concentrations and emissions of CH_4 from natural wetlands was simulated by a linear regression model. The results showed that the estimated annual budget of CH_4 emission from natural wetlands in the temperate zone of China was about 4.76 Tg CH_4, which was within the range of 2.38–4.91 Tg CH_4 estimated by spatial distribution of wetland and the published CH_4 release fluxes during the 1990s–2000s. This demonstrated that the method of using space-borne CH_4 column concentrations to estimate CH_4 emissions from natural wetlands was reliable.

14/01782 Impact of polycyclic aromatic hydrocarbon (PAH) emissions from North Korea to the air quality in the Seoul Metropolitan Area, South Korea
Kim, I. S. *et al. Atmospheric Environment*, 2013, 70, 159–165.
Due to its proximity to the Seoul Metropolitan Area (SMA) (40 km from Seoul proper to North Korea) and the characteristics of energy consumption (coal and biomass burning as major primary energy sources), air pollutants emitted from North Korea are likely to influence the air quality in the SMA. To understand the transport of air pollutants emitted from North Korea, backward trajectories arriving in Seoul were estimated and classified into four cases depending on which area the trajectories predominantly passed through for the sampling days between 2002 and 2003. The ambient data of particulate polycyclic aromatic hydrocarbons (PAHs) were analysed for the samples. Then, based on the contribution of biomass burning calculated by the chemical mass balance model applied and the influence of air pollutants' emissions from North Korea to SMA is semi-quantified. The result was verified by the spatial and seasonal variations of the PAH emission in China based on the previous works. It is estimated that the influence from North Korea on the particulate PAHs concentration in Seoul was up to 20% of the observed values. Further study directions are discussed to make more quantitative and reliable estimation.

14/01783 Improved CO, hydrocarbon and NO oxidation performance using zone-coated Pt-based catalysts

Abedi, A. *et al. Catalysis Today*, 2013, 207, 220–226.

The effect of an axial Pt distribution along a diesel oxidation catalyst (DOC) was investigated by comparing a standard catalyst, with a homogeneously distributed Pt amount along the length, with a non-homogeneously distributed catalyst (zoned). The zoned catalyst had more Pt located at the upstream portion, and less downstream, while maintaining the same total amount of Pt as the standard case. The effects of flow rate on NO, CO or C_3H_6 oxidation, and during oxidation of NO and C_3H_6 as a mixture, were used for the comparison. The reaction details along the catalyst were also resolved using spatially resolved, capillary inlet mass spectrometry (Spaci-MS). Results showed that the performance of the two catalysts were similar at low flow rate and with a single reacting gas, while the zoned sample worked better for CO and C_3H_6 oxidation as the flow rate increased, and better for NO oxidation in the NO/C_3H_6 gas mixture. With CO or C_3H_6 oxidation, the superior performance of the zoned sample was due to a larger, localized exotherm and a decreased self-poisoning effect. The exothermic heat produced in the front part of the zoned catalyst allowed it to reach higher temperature at the front faster than the homogeneous/standard sample and it also lowered the effect of self-poisoning by converting most of the reactants in the front part. NO oxidation, being kinetically more challenging, occurred along the entire length of catalyst at low temperature, not achieving near 100% conversion in these tests. Spatially resolved experiments during C_3H_6 and NO oxidation, as a mixture, showed that NO oxidation started after C_3H_6 was consumed. Therefore, for the zoned sample, C_3H_6 was oxidized closer to the inlet portion of the catalyst, where a higher density of Pt was located, leaving the rest of the catalyst available for NO oxidation. However, with the standard sample, C_3H_6 oxidation utilized a larger part of the catalyst leaving a smaller portion of the monolith for NO oxidation.

14/01784 Particle-bound polycyclic aromatic hydrocarbon concentrations in transportation microenvironments

Houston, D. *et al. Atmospheric Environment*, 2013, 71, 148–157.

This study is one of the first case studies to characterize the exposure of urban residents to traffic-related air pollution across locations and transportation microenvironments during everyday activities. Twenty-four adult residents of Boyle Heights, a neighbourhood near downtown Los Angeles, USA, carried a portable air pollution monitor and a global positioning systems tracking device for a total of 96 days. The authors found significant spatial and temporal variation in the particle-bound polycyclic aromatic hydrocarbon (pPAH) concentrations in transportation microenvironments. Average pPAH concentrations were higher while walking outdoors (190 ng m^{-3}) compared to travelling in private passenger vehicles (138–155 ng m^{-3}) or travelling in public transportation (61–124 ng m^{-3}). Although travel comprised 5% of participant days, it was associated with 27% of overall daily pPAH exposure. Regression models explained 40–55% of the variation in daily average pPAH concentrations, and 40–44% of the variation in 1-min interval concentrations. Important factors included time spent travelling, travel speed, meteorological and nearby land-use factors, time of day and proximity to roadways. Although future research is needed to develop stronger predictive models, this study demonstrates portable tracking devices can provide a more complete, diurnal characterization of air pollution exposures for urban populations.

14/01785 Pollution characteristics of volatile organic compounds, polycyclic aromatic hydrocarbons and phthalate esters emitted from plastic wastes recycling granulation plants in Xingtan Town, South China

Huang, D.-Y. *et al. Atmospheric Environment*, 2013, 71, 327–334.

With the aim to investigate the main pollution characteristics of exhaust gases emitted from plastic waste recycling granulation plants, mainly volatile organic compounds (VOCs), polycyclic aromatic hydrocarbons (PAHs) and phthalate esters (PAEs) were analysed in Xingtan Town, the largest distribution centre of plastic waste recycling in China. Both inside and outside the plants, the total concentrations of volatile monocyclic aromatic hydrocarbons (MAHs), PAHs and PAEs ranged from 2000 to 3000 μg m^{-3}, 450 to 1200 ng m^{-3} and 200 to 1200 ng m^{-3}, respectively. Their concentration levels inside the plants were higher than those outside the plants, and PAHs and PAEs were mainly distributed in the gas-phase. Notably, highly toxic benzo[a]pyrene (BaP) could be detected inside the plants, and harmful PAEs could be detected not only inside but also outside the plants, although PAEs are non-volatile. The exhaust gas composition and concentration were related to the plastic feedstock and granulation temperature.

14/01786 Predicting emissions of volatile and semivolatile organic compounds from building materials: a review

Liu, Z. *et al. Building and Environment*, 2013, 64, 7–25.

Volatile organic compounds (VOCs) and semivolatile organic compounds (SVOCs) constitute important classes of indoor air contaminants and characterizing their emissions from building materials and consumer products is of interest for risk assessment and the development of environmentally benign products. Compared with emission chamber studies, emission models provide a more cost effective and powerful way to examine the emission behaviour of VOCs and SVOCs. The objective of this paper is to review existing mechanistic models for predicting VOC and SVOC emissions from various sources, investigate their differences and similarities, and discuss the mass-transfer mechanisms on which the models are constructed. Because the usefulness of the emission models largely depends on the availability and reliability of model parameters, techniques for estimating key model parameters are also reviewed. The models covered in this review fall into three categories: models for VOC emissions from solid materials; models for VOC emissions from liquid materials; and models for SVOC emissions. VOC and SVOC emissions can be modelled within a consistent mass-transfer framework with the three model categories being intimately related. While substantial advances have been made in developing predictive models and understanding emission mechanisms, large knowledge gaps exist and further research is needed.

Life cycle analysis

14/01787 Addressing uncertainty in life-cycle carbon intensity in a national low-carbon fuel standard

Kocoloski, M. *et al. Energy Policy*, 2013, 56, 41–50.

Policies formulated to reduce greenhouse gas (GHG) emissions, such as a low-carbon fuel standard, frequently rely on life-cycle assessment (LCA) to estimate emissions, but LCA results are often highly uncertain. This study develops life-cycle models that quantitatively and qualitatively describe the uncertainty and variability in GHG emissions for both fossil fuels and ethanol and examines mechanisms to reduce those uncertainties in the policy process. Uncertainty regarding emissions from gasoline is non-negligible, with an estimated 90% confidence interval ranging from 84 to 100 g CO_2e/MJ. Emissions from biofuels have greater uncertainty. The widths of the 90% confidence intervals for corn and switchgrass ethanol are estimated to be on the order of 100 g CO_2e/MJ, and removing emissions from indirect land use change still leaves significant remaining uncertainty. Though an opt-in policy mechanism can reduce some uncertainty by incentivizing producers to self-report fuel production parameters, some important parameters, such as land use change emissions and nitrogen volatilization, cannot be accurately measured and self-reported. Low-carbon fuel policies should explicitly acknowledge, quantify, and incorporate uncertainty in life cycle emissions in order to more effectively achieve emissions reductions. Two complementary ways to incorporate this uncertainty in low carbon fuel policy design are presented.

14/01788 Carbon footprint evaluation at industrial park level: a hybrid life cycle assessment approach

Dong, H. *et al. Energy Policy*, 2013, 57, 298–307.

Industrial parks have become the effective strategies for government to promote sustainable economic development due to the following advantages: shared infrastructure and concentrated industrial activities within planned areas. However, due to intensive energy consumption and dependence on fossil fuels, industrial parks have become the main areas for greenhouse gas emissions. Therefore, it is critical to quantify their carbon footprints so that appropriate emission reduction policies can be raised. The objective of this paper is to seek an appropriate method on evaluating the carbon footprint of one industrial park. The tiered hybrid life cycle assessment method was selected due to its advantages over other methods. The Shenyang economic and technological development zone, a typical comprehensive industrial park in China, was chosen as a case study park. The results show that the total life cycle carbon footprint of the site was 15.29 Mt, including 6.81 Mt onsite (direct) carbon footprint, 8.47 Mt upstream carbon footprint, and only 3201 t downstream carbon footprint. Analysis from industrial sector perspectives shows that chemical industry and manufacture of general purpose machinery and special purposes machinery sector were the two largest sectors for life cycle carbon footprint. Such a sector analysis may be useful for investigation of appropriate emission reduction policies.

14/01789 Energy supply infrastructure LCA model for electric and hydrogen transportation systems

Lucas, A. *et al. Energy*, 2013, 56, 70–80.

Many transportation environmental life cycle analyses neglect the contribution of the energy supply infrastructures. In alternative light duty vehicle technologies, it has been shown through case studies that

this can be a relevant factor. However, no model that can generalize the evaluation of energy and emissions from construction, maintenance and decommissioning of such infrastructure to analyse different scenarios currently exists. A model is proposed, focusing on electricity and on hydrogen supply through centralized steam methane reforming (H_2(a)) and on-site electrolysis (H_2(b)). The model outputs are in gCO_{2eq}/MJ and MJ_{eq}/MJ of the final energy. Model main inputs are the region's electricity mix, the annual distance driven, supply chain losses and the number of vehicles per station or chargers. The evaluation of the number of vehicles served per each charger/station as a function of annual distance driven is presented. The uncertainty is estimated by using the pedigree matrix, impact uncertainty and literature estimates. The model shows consistency in the results and uncertainty range. Charging policies that minimize the electricity infrastructure burden should incentivize approximately 37% of normal charging. H_2(a) pipeline lifetime should be extended. Efforts in the electrolyser should be undertaken to approximate the ratio of vehicles per station with a conventional one.

14/01790 Evaluation of low grade heat transport in the process industry using absorption processes

Ammar, Y. *et al. Applied Thermal Engineering*, 2013, 53, (2), 217–225.
This paper looks at a long-distance heat transportation system based on an absorption process using a mixture of water and ammonia as a working fluid in order to use low-grade heat available in the process industry. This paper aims at establishing the potential of using this method for economically transferring low-grade heat from process industries to domestic heat sinks. To do so, the efficiency of transporting low-grade heat sources identified in the process industries was examined. The economic distance was defined as the limit for economically transferring low-grade heat from the source to the domestic heat sink. Based on a 10-year payback period, it was shown that heat could reach as far as 30–40 km for low grade heat sources at temperature as low as 80 °C. Finally, the economic distance was expressed as a function of the amount of fuel equivalent associated with low grade heat recovery savings and the economics of the transportation solution was discussed with regards to the expected changes of the heating and steel price over time.

14/01791 Life cycle analysis of fuel production from fast pyrolysis of biomass

Han, J. *et al. Bioresource Technology*, 2013, 133, 421–428.
A well-to-wheels (WTW) analysis of pyrolysis-based gasoline was conducted and compared with petroleum gasoline. To address the variation and uncertainty in the pyrolysis pathways, probability distributions for key parameters were developed with data from literature. The impacts of two different hydrogen sources for pyrolysis oil upgrading and of two bio-char co-product applications were investigated. Reforming fuel gas/natural gas for H_2 reduces WTW greenhouse gas emissions (GHG) by 60% (range of 55–64%) compared to the mean of petroleum fuels. Reforming pyrolysis oil for H_2 increases the WTW GHG emissions reduction up to 112% (range of 97–126%), but reduces petroleum savings per unit of biomass used due to the dramatic decline in the liquid fuel yield. Thus, the hydrogen source causes a trade-off between GHG reduction per unit fuel output and petroleum displacement per unit biomass used. Soil application of biochar could provide significant carbon sequestration with large uncertainty.

14/01792 Life cycle assessment of biochar cofiring with coal

Huang, Y.-F. *et al. Bioresource Technology*, 2013, 131, 166–171.
This study used the life cycle assessment software SimaPro 7.2 and the impact assessment model IMPACT 2002+ to evaluate the environmental impact and benefits of a biochar cofiring supply chain used for electricity generation. The biochar was assumed to be produced by rice straw torrefaction and the case study was located in Taoyuan County, Taiwan. This supply chain may provide impact reduction benefits in five categories (aquatic ecotoxicity, terrestrial ecotoxicity, land occupation, global warming and non-renewable energy) but cause higher impacts than coal firing systems in other categories. Damage assessment of cofiring systems indicated that damage to human health was higher while the damage categories of ecosystem quality, climate change, and resources were lower. Carbon reduction could be 4.32 and 4.68 tonnes CO_2 eq/ha/yr at 10% and 20% cofiring ratios, respectively. The improvement of electricity generation efficiency of cofiring systems may be the most important factor for reducing its environmental impact.

14/01793 Life cycle assessment of biohydrogen and biomethane production and utilisation as a vehicle fuel

Patterson, T. *et al. Bioresource Technology*, 2013, 131, 235–245.
Environmental burdens for the production and utilization of biomethane vehicle fuel or a biohydrogen/biomethane blend produced from food waste or wheat feed, based on data from two different laboratory experiments, have been compared. For food waste treated by batch processes the two stage system gave high hydrogen yields (84.21 $H_2\,kg^{-1}$ VS added) but a lower overall energy output than the single stage system. Reduction in environmental burdens compared with diesel was achieved, supported by the diversion of waste from landfill. For wheat feed, the semi-continuously fed two-stage process gave low hydrogen yields (7.51 $H_2\,kg^{-1}$ VS added) but higher overall energy output. The process delivers reduction in fossil fuel burdens, and improvements in process efficiencies will lead to reduction in CO_2 burdens compared with diesel. The study highlights the importance of understanding and optimizing biofuel production parameters according to the feedstock utilized.

14/01794 Life cycle assessment of rice straw co-firing with coal power generation in Malaysia

Shafie, S. M. *et al. Energy*, 2013, 57, 284–294.
This paper investigates the economic feasibility of rice straw co-firing at coal power plants in Malaysia and in doing so looks at the operating, capital and logistic costs. Co-firing rice straw in an existing coal power plant is a technique that could reduce CO_2 emissions and make Malaysia less dependent on coal resources. In a country such as Malaysia with abundant biomass resources, using biomass residue also would help reach government targets of developing renewable energy under the country's fuel diversification policy. The overall rice straw life cycle assessment presented here analyses environmental, energy and economic aspects for co-firing of rice straw at existing coal power plants in Malaysia. Analysis of greenhouse gas (GHG) emissions and energy consumption throughout the entire co-firing rice straw life cycle was based on selected coal power plant capacity output. This paper also analyses the implication of rice straw use under different co-fired ratios, transportation systems and CO_2 emission prices. The reduction of GHG emissions was found to be significant even at a lower co-firing ratio.

14/01795 Life-cycle energy efficiency and environmental impacts of bioethanol production from sweet potato

Wang, M. *et al. Bioresource Technology*, 2013, 133, 285–292.
Life-cycle assessment (LCA) was used to evaluate the energy efficiency and environmental impacts of sweet potato-based bioethanol production. The scope covered all stages in the life cycle of bioethanol production, including the cultivation and treatment, transport, as well as bioethanol conversion of sweet potato. Results show that the net energy ratio of sweet potato-based bioethanol is 1.48 and the net energy gain is 6.55 MJ/L. Eutrophication is identified as the most significant environmental impact category, followed by acidification, global warming, human toxicity, and photochemical oxidation. Sensitivity analysis reveals that steam consumption during bioethanol conversion exerts the most effect on the results, followed by sweet potato yields and fertilizers input. It is suggested that substituting coal with cleaner energy for steam generation in bioethanol conversion stage and promotion of better management practices in sweet potato cultivation stage could lead to a significant improvement of energy and environmental performance.

14/01796 Practical ambiguities during calculation of energy ratios and their impacts on life cycle assessment calculations

Zhang, Y. and Colosi, L. M. *Energy Policy*, 2013, 57, 630–633.
The energy ratio metrics are increasingly important means of assessing the efficiency of energy production for emerging biofuels platforms, making comparisons among multiple alternatives, and formulating policies to foster commercialization of sustainable energy systems. However, these metrics are susceptible to inadvertent or meaningful mathematical manipulation, whereby the same dataset can be used to compute dramatically different values of energy return on investment (EROI). In this study, previously published life cycle assessment (LCA) data for algal biofuels, corn ethanol, and switchgrass ethanol are used to demonstrate how seven seemingly reasonable EROI formulations give rise to a wide range of output values. It is then demonstrated that production of bioelectricity, and to a lesser extent, other co-products, significantly increases EROI ambiguity. Overall, the EROI results are used to illustrate how EROI ambiguity makes it difficult to properly assess the energetic favourability of a particular energy system or to make accurate comparisons among multiple systems. It is then recommended that all future biofuels studies restrict themselves to usage of '$EROI_1$', which documents all input and outputs as explicit terms, to mitigate EROI ambiguity and improve policy decision-making.

14/01797 The environmental impact of organic Rankine cycle for waste heat recovery through life-cycle assessment

Liu, C. *et al. Energy*, 2013, 56, 144–154.
Life-cycle assessment (LCA) was applied to evaluate the environmental impact of an organic Rankine cycle power-plant for waste-heat-recovery (ORCPW) in this paper. The model of LCA on the ORCPW was established. The life-cycle of ORCPW was divided into construc-

tion, operation and decommissioning phases. The inventory of environmental emissions was listed for the ORCPW with seven different working fluids. The global warming potential (GWP), acidification potential, eutrophication potential, human toxicity potential (HTP), solid waste potential, and soot and dust potential were investigated. Some environmental impacts of ORCPW were compared with the environmental impacts of other power generation modes. The results show that the construction phase of ORCPW contributes mostly to the GWP and eutrophication potential. GWP is the most serious environmental impact followed by HTP among all the environmental impacts. The average payback times of greenhouse gases discharged from ORCPW are calculated on the basis of five other power generation modes. For seven different working fluids it is 3–5 years for CO_2, about one year for CH_4 and 3–6 years for NO_x. But CO cannot be paid back during the life-cycle of ORCPW according to the average payback time.

16 ENERGY

Supplies, policy, economics, forecasts

14/01798 A modified GHG intensity indicator: toward a sustainable global economy based on a carbon border tax and emissions trading

Moghaddam, R. F. *et al. Energy Policy*, 2013, 57, 363–380.

It will be difficult to gain the agreement of all the actors on any proposal for climate change management, if universality and fairness are not considered. In this work, a universal measure of emissions to be applied at the international level is proposed, based on a modification of the greenhouse gas intensity (GHG-INT) measure. It is hoped that the generality and low administrative cost of this measure, called here the modified greenhouse gas intensity measure (MGHG-INT), will eliminate any need to classify nations. The core of the MGHG-INT is called here the IHDI-adjusted gross domestic product (IDHIGDP), based on the inequality-adjusted human development index (IHDI). The IDHIGDP makes it possible to propose universal measures, such as MGHG-INT. The authors also propose a carbon border tax applicable at national borders, based on MGHG-INT and IDHIGDP. This carbon tax is supported by a proposed global emissions trading system. The proposed carbon tax is analysed in a short-term scenario, where it is shown that it can result in a significant reduction in global emissions while keeping the economy growing at a positive rate. In addition to annual GHG emissions, cumulative GHG emissions over two decades are considered with almost the same results.

14/01799 Analysis of energy embodied in the international trade of UK

Tang, X. *et al. Energy Policy*, 2013, 57, 418–428.

Interest in the role embodied energy plays in international trade and its subsequent impact on energy security has grown. As a developed nation, the UK's economic structure has changed from that of a primary producer to that of a primary consumer. Although the UK's energy consumption appears to have peaked, it imports a lot of energy embodied in international trade alongside the more obvious direct energy imports. The UK has seen increasing dependency on imported fossil energy since the UK became a net energy importer in 2005. In this paper an energy input–output model is established to calculate not only the amount of fossil energy embodied in UK's imports and exports, but also the sector and country distributions of those embodied fossil energy. The research results suggest the following: UK's embodied fossil energy imports have exceeded embodied fossil energy exports every year since 1997, UK embodied energy imports through the so-called 'Made in China' phenomena are the largest accounting for 43% of total net fossil energy imports. If net embodied fossil energy imports are considered, the gap between energy consumption and production in UK is much larger than commonly perceived, with subsequent implications to the UK's energy security.

14/01800 Ecuador's energy policy mix: development versus conservation and nationalism with Chinese loans

Escribano, G. *Energy Policy*, 2013, 57, 152–159.

Ecuador's energy policy faces a complex variety of political and economic objectives that are difficult to reconcile in a consistent manner. Ecuador is a small oil producer and exporter with significant renewable (mainly hydropower) resources, hosting some of the richest biodiversity areas in the world, part of which are inhabited by so far indigenous un-contacted people. Being a developing country, tensions arise between conservation aims and development imperatives, as well as between resource nationalism and much-needed foreign financing. However, the really limiting factor for the country's energy development seems to be its constraints in financing the government's development and redistributive policies. Resorting to Chinese loans-for-oil may be part of the solution in the short term, but it does not substitute for a more consistent energy policy. Ecuador's case illustrates the dilemmas of energy policy in natural resource-rich developing countries when confronted with diverging political economy, social, environmental and macro-financial goals.

14/01801 Energy performance of low temperature heating systems in five new-built Swedish dwellings: a case study using simulations and on-site measurements

Hesaraki, A. and Holmberg, S. *Building and Environment*, 2013, 64, 85–93.

In Europe, high energy consumption in built environments has raised the need for developing low energy heating systems both in new building and in retrofitting of existing buildings. This paper aims to contribute by presenting annual results of calculated and measured energy consumption in five new-built semi-detached dwellings in Stockholm, Sweden. All buildings were equipped with similar low temperature heating systems combining under-floor heating and ventilation radiators. Exhaust ventilation heat pumps supported the low temperature heating system. Buildings were modelled using an energy simulation tool and energy consumption of the heat pumps was measured. Results showed that calculated and measured results were generally in agreement for all five dwellings, and that the buildings not only met energy requirements of the Swedish building regulations but also provided good thermal comfort.

14/01802 EU and Russian discourse on energy relations

Kratochvíl, P. and Tichý, L. *Energy Policy*, 2013, 56, 391–406.

The paper explores the dominant interpretations of the European Union (EU)–Russian energy relations by identifying three dominant concepts around which these interpretations revolve: (1) integration, (2) liberalization and (3) diversification. Building on a detailed discourse analysis of 97 textual units produced by EU leaders and institutions and 104 documents and speeches by Russian policy-makers, the paper argues that these three discourses differ widely in their assessment of the two partners' mutual ties, both in terms of the relationship's symmetry and the perceived benefits for each partner. The paper comes up with two basic arguments. First, in spite of the shared usage of the three basic notions by both sides, the interpretations of each of the discourses are widely different in the EU and in Russia, which causes continuous frictions and misunderstandings. Second and surprisingly, the discourse of integration is dominant both in the EU and Russia, which shows that the claims about the alleged securitization of EU–Russian energy relations are clearly exaggerated.

14/01803 Forecasting long-term energy demand of Croatian transport sector

Pukšec, T. *et al. Energy*, 2013, 57, 169–176.

The transport sector in Croatia represents one of the largest consumers of energy today, with a share of almost one-third of the country's final energy demand. Considering this fact, it is very challenging to assess future trends influencing that demand. In this paper, long-term energy demand predictions for the Croatian transport sector are presented. Special emphasis is given to different influencing mechanisms, both legal and financial. The energy demand predictions presented in this paper are based on an end-use simulation model developed and tested with Croatia as a case study. The model incorporates the detailed modal structure of the Croatian transport sector, including road, rail, air, public and water transport modes. Four long-term energy demand scenarios were analysed until the year 2050; frozen efficiency, implementation of European Union legislation, electrification and modal split. Based on that analysis, significant savings can be achieved through energy efficiency improvements, electrification of personal vehicles fleet as well as gradual modal split. Comparing the frozen efficiency scenario and electrification scenario for the year 2050, it can be concluded that energy consumption, with the heavy electrification of personal vehicles fleet, can be cut by half.

14/01804 GIS based analysis of future district heating potential in Denmark

Nielsen, S. and Möller, B. *Energy*, 2013, 57, 458–468.

The physical placement of buildings is important when determining the potential for district heating (DH). Good locations for DH are mainly determined by having both a large heat demand within a certain area and having access to local heat resources. In recent years, the locations of buildings in Denmark have been mapped in a heat atlas which includes all buildings and their heat demands. This paper focuses on developing a method for assessing the costs associated with supplying these buildings with DH. The analysis is based on the existing DH areas in Denmark. By finding the heat production cost within these areas and

adding transmission and distribution costs, it is possible to find the economic feasibility of supplying areas with DH. The findings of the analysis indicate that there is potential for expanding DH in Denmark, but this potential differs from area to area. It is economically feasible to expand DH in many areas, but others would require reductions in production costs and distribution losses in order for DH expansions to be economically feasible. The analysis also shows the potential boundaries for DH expansion by including transmission and distribution costs. These boundaries are not static, but change according to many different factors.

14/01805 Modelling and mapping sustainable heating for cities

Finney, K. N. *et al. Applied Thermal Engineering*, 2013, 53, (2), 246–255.

Decentralized energy in the UK is rare. Cities in the north of England however lead the UK in terms of sustainable, low-carbon, local/district heating, through the implementation of combined-heat-and-power (CHP) facilities; substantial schemes are installed in several cities, including Barnsley and Sheffield. This paper presents the results from extensive experimental and theoretical feasibility studies, in which the merits of these were explored. Barnsley has a number of biomass-fuelled community energy generators, where pollutant monitoring and mathematical modelling were conducted to assess combustion characteristics and overall system performance. Measured pollutant levels were within the relative emission limits, though emission concentrations (CO, CO_2, NO and particles) in the flue gas from the coal boiler were higher than the wood pellet boiler. Sheffield already has a citywide district energy network, centred around a sustainably sourced waste-to-energy facility; an expansion of this scheme was investigated here. This focuses mainly on the link to a 30 MW wood-fired CHP plant, which could be a significant provider of additional thermal capacity (low-grade heat) to an expanded network. Through identifying heat sources and sinks – potential suppliers and end-users – key areas were identified where a connection to the heat network would be feasible.

14/01806 Multicriteria analysis for the assessment of energy innovations in the transport sector

Scarpellini, S. *et al. Energy*, 2013, 57, 160–168.

In the current context of environmental and global challenges, eco-innovation has become one of the European Union's priorities. A proper measurement system is a need for the promotion, long-term decision making and progress assessment of eco-innovative activities. Public and private sectors have to refocus their activities in order to pursue maximum profits, not only economic but social and environmental. Conventional indicators and metrics for innovation measurement are not suitable because they do not take into account these three dimensions of the sustainability in a balanced analysis. After identifying the minimum requirements of a method for measuring eco-innovation, a simplified multi-criteria analysis based on saving-investment curves is proposed and applied to the transport sector. This approach is suitable to determine how actions should be prioritized providing the basis for further assessments.

14/01807 The industrial logistic surface: displaying the impact of energy policy on uptake of new technologies

Mathews, J. A. and Baroni, P. *Energy*, 2013, 57, 733–740.

Two processes are widely viewed as fundamental to the transition from conventional fossil-fuelled energy systems to renewable powered systems that is under way. There is firstly the progressive reduction in costs as investment, or production/energy generating capacity, grows. To see the uptake itself a second process is needed, captured as a logistic curve (or S-shaped curve) that depicts the uptake of the new technology as an industrial substitution process unfolding over time. This paper puts these two processes together, deriving a single expression that depicts uptake as a function of both cumulative investment and time, where the key parameter can be related to the learning coefficient. This expression is displayed in the form of a three-dimensional surface dubbed the logistic industrial surface. It is applied to a real case involving cost reduction and logistic uptake of solar photovoltaic cells. In this specific case, the authors estimate the learning curve involved and on this basis calculate that (for an initial time period) early in the trajectory a cost reduction of 8.7% would be associated with an increase in investment of 10%, leading to an increase in uptake by 4.35%; whereas a cost reduction of 44% (corresponding to a doubling of investment) would lead to a more rapid uptake of 41.95%. The authors claim that this is the first demonstration in the literature of a direct connection between investment levels, cost reductions and consequent levels of uptake according to logistic industrial dynamics.

14/01808 The influence of energy consumption of China on its real GDP from aggregated and disaggregated viewpoints

Zhang, W. and Yang, S. *Energy Policy*, 2013, 57, 76–81.

This paper investigated the causal relationship between energy consumption and gross domestic product (GDP) in China at both aggregated and disaggregated levels during the period of 1978–2009 by using a modified version of the Granger causality test within a multivariate framework. The empirical results suggested the existence of a negative bidirectional Granger causality running from aggregated energy consumption to real GDP. At disaggregated level of energy consumption, the results were complicated. For coal, empirical findings suggested that there was a negative bidirectional Granger causality running from coal consumption to real GDP. However, for oil and gas, empirical findings suggested a positive bidirectional Granger causality running from oil as well as gas consumption to real GDP. Though these results supported the feedback hypothesis, the negative relationship might be attributed to the growing economy production shifting towards less energy intensive sectors and excessive energy consumption in relatively unproductive sectors. The results indicated that policies with reducing aggregated energy consumption and promoting energy conservation may boost China's economic growth.

14/01809 The strategic interaction between the government and international oil companies in the UK: an example of a country with dwindling hydrocarbon reserves

Willigers, B. J. A. and Hausken, K. *Energy Policy*, 2013, 57, 276–286.

The 2011 UK tax rise on hydrocarbon exploitation activities obviously increases short-term tax revenues however the longer term effects are less clear. The strategic interaction between the UK government, a producer and a shipper has been analysed in a game theoretical model. A complex interaction between players is expected given: (1) dwindling resources and large decommissioning liabilities and (2) the fact that much of the hydrocarbons produced in the North Sea are exported through an infrastructure with shared ownership. The 2011 UK tax adjustment will most likely result in value destruction for the government, producers and shippers. This analysis suggests that governments are unlikely to ultimately benefit from reducing their decommission liabilities at the expense of international oil companies. In countries with unstable tax regimes, such as the UK, international oil companies will adopt their strategies in anticipation of future tax changes. Their adopted strategy is a function of decommissioning liabilities and remaining reserves as well as whether they are producers, shippers or producers and shippers. The ultimate payoff of a government is a function of the remaining reserves and total decommissioning liabilities, but also depends on the distribution of these value metrics between producers and shippers.

14/01810 Towards nearly zero-energy buildings: the state-of-art of national regulations in Europe

Annunziata, E. *et al. Energy*, 2013, 57, 125–133.

Energy efficiency in buildings is an important objective of energy policy and strategy in Europe. A survey questionnaire was conducted among the 27 European Union member states. This study aims to provide an overview of the current national regulatory framework focusing on three aspects: (1) integration of energy efficiency and renewable energy requirements, (2) translation of investments in energy saving into economic value and (3) commitment towards 'nearly zero-energy' target. The study shows that European countries have adopted different approaches in the design of their national regulatory framework. This heterogeneity consists of four main factors: different authorities involved in energy regulations, traditional building regulations and enforcement models, different contextual characteristics, and maturity of the country in the implementation of energy efficiency measures. These differences are important to take into account country's profile in order to improve the sharing of best-practices and energy efficiency governance among European Union member states.

14/01811 Waste oil derived biofuels in China bring brightness for global GHG mitigation

Liang, S. *et al. Bioresource Technology*, 2013, 131, 139–145.

This study proposed a novel way for global greenhouse gas reduction through reusing China's waste oil to produce biofuels. Life cycle greenhouse gas mitigation potential of aviation bio-kerosene and biodiesel derived from China's waste oil in 2010 was equivalent to approximately 28.8% and 14.7% of mitigation achievements on fossil-based CO_2 emissions by Annex B countries of the Kyoto Protocol in the period of 1990–2008, respectively. China's potential of producing biodiesel from waste oil in 2010 was equivalent to approximately 7.4% of China's fossil-based diesel usage in terms of energy. Potential of aviation bio-kerosene derived from waste oil could provide about 43.5% of China's aviation fuel demand in terms of energy. Sectors key to waste oil generation are identified from both production and consumption perspectives. Measures such as technology innovation, government supervision for waste oil collection and financial subsidies should be introduced to solve bottlenecks.

Energy conservation

14/01812 Building energy saving potential in hot summer and cold winter (HSCW) zone, China – influence of building energy efficiency standards and implications

Xu, L. *et al. Energy Policy*, 2013, 57, 253–262.

The hot summer and cold winter (HSCW) region plays an important role in China's building energy conservation task due to its high consumption in recent years for both climate and social reasons. National and local building energy standards according to which the buildings are built and operated can affect the building energy consumption to a great extent. This study investigated the energy saving potential in hot summer and cold winter zone under different level of energy efficiency standards (China local, China national and UK standard). Chongqing was taken as an example, and the commercial energy simulation tool eQuest was applied to analyse the building end-use energy. With the existing situation as a baseline, the building energy saving for residential section could achieve 31.5% if the Chinese national standard were satisfied, and the value would further increase to 45.0% and 53.4% when the Chongqing local and UK standard were met. For public buildings, the corresponding energy saving potentials were 62.8%, 67.4% and 75.9%. Parameter sensitivity analysis was conducted. The analysis was able to provide suggestions on energy saving implementation priorities for residential and public buildings. Indications to improve building energy standards and their implementation were also discussed.

14/01813 Chinese consumer attitudes towards energy saving: the case of household electrical appliances in Chongqing

Ma, G. *et al. Energy Policy*, 2013, 56, 591–602.

Energy saving is now an important component of China's energy policy. This paper reports the findings of a survey carried out in 2009 and 2010 of 246 citizens at different locations in the municipality of Chongqing in order to reveal information about attitudes towards energy and energy saving in the context of household electrical appliances. This study shows that citizens in Chongqing receive relatively little information and guidance on how to save energy in the home and that their stated level of knowledge on this subject is also rather limited. Respondents showed some willingness to save energy as long as this did not reduce their comfort and convenience, and they appeared likely to respond to economic incentives, such as high electricity prices or discounts on appliances. But they seemed to be unaware of the potential for information to help them save energy. The survey also demonstrated a high degree of heterogeneity across society with respect to sources of information and trust in those sources and with respect to attitudes to energy saving at home. These results show that the government needs to substantially adjust its strategies for promoting household energy saving.

14/01814 Current situations and technical development of energy-savings in China refrigeration industries

Wu, S. *et al. Applied Thermal Engineering*, 2013, 53, (2), 271–277.

The promotion of energy efficiency standards and the implementation of energy labels have greatly improved energy efficiencies of Chinese refrigeration products in recent years. These products are now moving towards multiple heat sources and multiple functions, to obtain further energy-savings. Some typical products, such as solar energy refrigerators and air conditioning-water heater system are introduced. The current energy efficiencies of Chinese refrigeration products are also introduced in this paper. Some recommendations are given to make the standards accommodate these changes.

14/01815 Energy conservation in China's higher education institutions

Lo, K. *Energy Policy*, 2013, 56, 703–710.

This paper analyses the energy conservation situation in China's higher education institutions (HEIs). A case study was conducted in Changchun, Jilin, where eight HEIs of various types were examined. An analysis of government policies was also performed. The findings indicate that the HEIs have implemented comprehensive non-technical initiatives to conserve electricity, including electricity restrictions and extensions of winter breaks, as well as certain technical initiatives. The HEIs are less enthusiastic in conserving thermal energy due to a lack of financial incentives and resources. Differences between the HEIs are also noted. This paper discusses the role of key players, including administrators, government agencies, networks, students and non-government organizations. Challenges to energy conservation are also identified, such as the lack of investment by schools, lack of government funding, quality problems in energy conservation products, inadequate heat metering reform, underperformance of energy service companies, and conflicts between energy conservation and student welfare. Policy recommendations are offered based on the analysis results.

14/01816 Energy consumption and economic analyses of a district heating network

Pirouti, M. *et al. Energy*, 2013, 57, 149–159.

An approach for minimization of the capital costs and energy consumption in a district heating network is presented using a case study based on a district heating network in south Wales, UK. A number of different design cases were simulated using the PSS SINCAL, taking into account different supply and return temperatures and target pressure losses. The operation of the district heating network was synthesized under different design cases using four district heating operating strategies. Optimization was conducted to obtain the optimal flow rate and supply temperature for the variable flow and variable supply temperature operating strategy. The optimization model was formulated using the FICO™ Xpress optimization suite. The objective of optimization was to minimize the annual total energy consumption and costs. Using each operating strategy, the annual pump energy consumption, heat losses and the equivalent annual cost were found and compared. A variable flow and variable supply temperature operating strategy was found to be beneficial in all cases. Design cases with minimum annual total energy consumption and cost used small pipe diameters and large pressure drops. Further, by increasing temperature difference between supply and return pipes, the annual total energy consumption and the equivalent annual cost were reduced.

14/01817 Energy consumption feedback devices' impact evaluation on domestic energy use

Vassileva, I. *et al. Applied Energy*, 2013, 106, 314–320.

Household energy accounts for one of the major contributors to the countries energy balances. It has been shown, that an effective way to achieve energy saving in that sector, is by providing consumers with information and feedback. This measure increases home inhabitants' awareness that leads to behavioural changes, and could help reduce energy consumption between 15% and 25% in some cases. Inhabitants' energy use awareness is also crucial for the success of demand response programmes; one of the most important features of smart-grid adoption for the current and upcoming smart cities. The effects of different feedback strategies and information devices in households located in different cities in Sweden have been evaluated in this paper, since the impact on users' behaviour of this feedback information vary depending on the way it is provided. Mobile text messages and digital displays placed in the building's common areas did not cause any noticeable behavioural changes, while the use of a TV channel and personal in-home displays were the most popular devices amongst households with high incomes. This paper concluded that even though feedback helped reduce domestic energy consumption and induce behavioural changes, it only reaches the consumers interested in it. It is important therefore to provide customized information to the consumer and select precise feedback tools for specific household groups. Special attention should be paid to increasing the energy consumption awareness in households with low income levels.

14/01818 For better or for worse? Empirical evidence of moral licensing in a behavioral energy conservation campaign

Tiefenbeck, V. *et al. Energy Policy*, 2013, 57, 160–171.

Isolated environmental campaigns focusing on defined target behaviours are rolled out to millions of households every year. Yet it is still unclear whether these programs trigger cross-domain adoption of additional environment-friendly behaviours (positive spillover) or reduced engagement elsewhere. A thorough evaluation of the real net performance of these programs is lacking. This paper investigates whether positive or perverse side effects dominate by exemplifying the impact of a water conservation campaign on electricity consumption. The study draws on daily water (10,780 data points) and weekly electricity (1386 data points) consumption data of 154 apartments in a controlled field experiment at a multifamily residence. The results show that residents who received weekly feedback on their water consumption lowered their water use (6.0% on average), but at the same time increased their electricity consumption by 5.6% compared with control subjects. Income effects can be excluded. While follow-up research is needed on the precise mechanism of the psychological process at work, the findings are consistent with the concept of moral licensing, which can more than offset the benefits of focused energy efficiency campaigns, at least in the short-term. The adoption of a more comprehensive view in environmental program design/evaluation is advocated in order to quantify and mitigate these unintended effects.

14/01819 Optimising entire lifetime economy of heat exchanger networks

Nemet, A. *et al. Energy*, 2013, 57, 222–235.

This contribution presents an optimization methodology for a heat exchanger network (HEN) design over its entire lifespan. Consideration of fluctuating energy prices is essential for achieving an optimal HEN design. The objective function presents a trade-off between investment and operating costs. Accounting for higher energy prices supports greater investments compared to solutions obtained with current prices. However, due to the uncertainty of utility prices' forecasts, retrofit with the extension of HEN regarding the lifespan, will usually be the future strategy. As there can be various designs featuring similar initial investments, the objective is to identify one design that will be the most suitable for effective future extensions, preferably with low sensitivity to energy price fluctuations. These observations resulted in development of a stochastic multi-period mixed-integer non-linear programming model for the synthesis of HEN designs, with extensions accounting for future energy prices. The objective of this work was to maximize both the expected net present value with no risk assessment performed, and the certainty equivalent with risk assessment regarding future utility prices and investment. The results obtained indicate that when applying the proposed approach, a design with improved economic performance could be obtained, especially when compared with total annual cost.

14/01820 Rewarding energy savings rather than energy efficiency: exploring the concept of a feed-in tariff for energy savings

Bertoldi, P. *et al. Energy Policy*, 2013, 56, 526–535.

Financial incentives are important for overcoming certain market barriers to improved energy efficiency and for the adoption of energy efficient technologies. Financial incentives are mainly focused on the introduction of specific technologies, rather than behavioural change. While the declared goal of financial support schemes very often is to save energy or reduce harmful emissions rather than to foster new technologies *per se*, it is often encountered that such financial support for energy efficient technologies may not ensure real energy savings due to the rebound effect and various market barriers. In the area of renewable energies it is common for financial support to be given to power producers for the verified production of renewable electricity, in the form of a guaranteed financial incentive (feed-in tariff). In the energy efficiency policy research little attention has been paid to the possible use of a 'feed-in tariff' in the form of a financial incentive based on the kWh saved by the end-user. This paper discusses the possible setup of a feed-in tariff designed to reward energy savings.

14/01821 Simultaneous optimization of propeller–hull systems to minimize lifetime fuel consumption

Nelson, M. *et al. Applied Ocean Research*, 2013, 43, 46–52.

In traditional naval architecture design methodologies optimization of the hull and propeller are done in two separate phases. This sequential approach can lead to designs that have sub-optimal fuel consumption and, thus, higher operational costs. This work presents a method to optimize the propeller–hull system simultaneously in order to design a vessel to have minimal fuel consumption. The optimization uses a probabilistic mission profile, propeller–hull interaction, and engine information to determine the coupled system with minimum fuel cost over its operational life. The design approach is tested on a KCS SIMMAN container ship using B-series propeller data and is shown to reduce fuel consumption compared to an optimized traditional design approach.

14/01822 Spatial planning framework for biomass resources for power production at regional level: a case study for Fujian Province, China

Sun, Y. *et al. Applied Energy*, 2013, 106, 391–406.

Effective spatial planning is crucial for cost-effectively and sustainably developing biomass energy resources due to the diffuse nature of biomass and high transportation cost. Using the spatial analysis technology, economic models and scenario analysis, this paper presents a spatial planning framework to identify the appropriate developing areas of biomass energy at regional level. The methodology is applied in a case study of Fujian Province, China. First, spatial distribution of two kinds of biomass resources and the technical potential, i.e. the amount of power generation from agricultural and forestry residues in each supply area, were estimated by incorporating the spatial data and the statistical data. The results indicate that total technical potential of agricultural and forestry residues is estimated at $25.13\,\mathrm{TW\,h\,y^{-1}}$, equivalent to approximately 19% of total electricity consumption in Fujian in 2010. In the second step, the economic analysis assesses the cost of biomass generation for each supply area on the basis of current market conditions. Ranking of the supply areas is then performed by using the priority development index (PDI), which can measure the priority of each biomass supply area by combining several influencing indicators. Finally, the selection of supply areas for power plants can be carried out according to its order in PDI until the total planed capacity in the region is met. The priority of the subregions and the corresponding cost of biomass generation for different planning scenarios can be explicitly visualized. The methodology can be applied to a wide area and can support the local authorities to define and implement a strategy for future biomass energy development.

14/01823 The effect of improved efficiency on energy savings in EU-27 buildings

Broin, E. Ó. *et al. Energy*, 2013, 57, 134–148.

Using energy efficiency techniques to lower energy demand in buildings is a key policy goal of the European Commission (EC). This paper presents the results of bottom-up modelling to elucidate the impact of energy efficiency on the European Union (EU) building stock up to 2050 under three different scenarios. The modelling is performed for eight individual EU countries and a ninth hypothetical entity that represents the remaining 19 EU countries. The scenarios highlight the roles of different levels of efficiency improvements in the context of increasing floor area and the demand for energy services. From the results it can be concluded that the EC 2020 goals for primary energy savings can be met by focusing on a combination of minimum efficiency construction standards, improved conversion efficiency standards for final energy to useful energy, and a $\geq$2% annual improvement in end-use efficiency applied at the useful energy level. A comparison of the results obtained in the present study for Spain with the estimates of savings documented in the Spanish Energy Efficiency Action Plan indicate that the plan could lead to the closing of the energy efficiency gap for buildings in that country by 2020.

14/01824 Use of electromagnetic clutch water pumps in vehicle engine cooling systems to reduce fuel consumption

Shin, Y. H. *et al. Energy*, 2013, 57, 624–631.

In general, when the internal combustion engine of a vehicle is started, its operationally connected cooling system provides excessive cooling, resulting in unnecessary energy consumption and excessive emission of exhaust gas. If the rotational speed of the engine is high, the excessive cooling causes the combustion efficiency to decrease. Therefore, better control of the operating temperature range of the engine through use of an active cooling system can achieve better fuel economy and reduction of exhaust gas emission. Effective control of the cooling system in accordance with the operating conditions of the engine can be realized by changing the mass flow rate of the coolant. In this study, electromagnetic clutch water pumps that can control the coolant flow were designed. Two types of water pump were made: (1) a planetary gear (PG)-type water pump which can reduce the rotation speed of the water pump by 65%, compared with a pulley; and (2) an on/off-type water pump which can completely stop the rotation of the impeller. The performance evaluation of these pumps consisted of a warm-up test and the New European Driving Cycle (NEDC). Warm-up test results showed that the time required to achieve a temperature of approximately 80 °C with the PG water pump and the on/off water pump was improved by 7.3% and 24.7% respectively, compared with that of a conventional water pump. Based on the NEDC results, the authors determined that the fuel economy of the engine using the PG water pump and the on/off water pump was improved by 1.7% and 4.0% compared with the fuel economy when using the conventional water pump. The application of clutch water pumps is expected to contribute to the improvement of engine cooling system performance, because their effect in reducing the fuel consumption rate is similar to that of an electric water pump.

17 ENERGY CONVERSION AND RECYCLING

14/01825 A novel conical combustor for thermal exploitation of vineyard pruning wastes

San José, M. J. *et al. Fuel*, 2013, 110, 178–184.

In order to determine the behaviour of a new conical spouted bed combustor for the thermal exploitation of vineyard pruning wastes by combustion, a hydrodynamic study has been carried out with homogenous beds wastes of pruning of vineyards, the evolution of the different regimes and the stable operation conditions have been determined. Beds consisting of vine shoots have been dried for improving combustion. The success of the combustion of wastes of vineyards pruning in a conical spouted bed combustor has been proven based on combustion efficiency values.

14/01826 Advantages of syngas for the regeneration of NO_x trap system investigated with *operando* IR measurements

Dujardin, C. *et al. Catalysis Today*, 2013, 205, 10–15.

The regeneration of a lean NO_x trap catalyst (Pt–Rh/BaO–Al_2O_3) using $H_2 + CO$ was followed with the *operando* infrared (IR) spectroscopy methodology. The role of H_2 was investigated from 2 to 20 vol.% H_2. The increase of H_2 partial pressure allowed a subsequent decrease of the regeneration duration. The quantity of NH_3 formed during the regeneration was related to H_2 quantity which suggests that NH_3 formation is governed by the supply of H_2. The reactivity of nitrate was found to be slower than that of nitrite species towards hydrogen at 250 °C. CO addition strongly inhibited ammonia production at 150 °C due to an accumulation of carbonate species at the surface of the catalyst. Above 250 °C, two processes coexisted for the reduction of NO_x into ammonia in the presence of the $H_2 + CO$ mixture: the successive hydrogenation of N atoms from NO dissociation and the hydrolysis of isocyanate species was evidenced by IR.

14/01827 Exergy efficiency enhancement of MSF desalination by heat recovery from hot distillate water stages

Al-Weshahi, M. A. *et al. Applied Thermal Engineering*, 2013, 53, (2), 226–233.

This detailed exergy analysis of a 3800 m^3/h multi-stage flash (MSF) desalination plant is based on the latest published thermodynamic properties of water and seawater. The parameters of the study were extracted from a validated model of MSF desalination using IPSEpro software. The results confirmed that the overall exergy efficiency of the unit is lower than would be desirable at only 5.8%. Exergy inputs were destroyed by 55%, 17%, 10%, 4.3% and 14%, respectively, in the heat recovery stages, brine heater, heat rejection stages, pumps and brine streams disposal. Moreover, the detail of the study showed that the lowest exergy destruction occurs in the first stage, increasing gradually in heat recovery stages and sharply in heat rejection stages. The study concludes that recovering the heat from the hot distillate water stages can improve unit exergy efficiency from its low 5.8% to a more economical 14%, with the hot water parameters suitable for powering other thermal systems such as absorption chiller and multi-effect desalination.

14/01828 Improving biodiesel yields from waste cooking oil using ionic liquids as catalysts with a microwave heating system

Lin, Y.-C. *et al. Fuel Processing Technology*, 2013, 115, 57–62.

Biodiesel made from waste cooking oil (WCO) can be used to effectively reduce the raw material cost as well as solve the problem of waste oil disposal. This study investigates the use of the ionic liquid 4-allyl-4-methylmorpholin-4-ium bromine (IL; [MorMeA][Br]) as a catalyst and a microwave heating system for improving biodiesel yields from WCO. Experimental results indicate that [MorMeA][Br] catalysts can increase WCO biodiesel yields and decrease the use of NaOH catalysts by 0.25 wt%. The best yield of WCO biodiesel is 89.1% under a $IL_1NaOH_{0.75}$ catalyst (1 wt% [MorMeA][Br] + 0.75 wt% NaOH), a methanol-to-oil molar ratio of nine, a reaction time of 6 min, and a microwave temperature of 70 °C. The IL catalyst was recyclable and thermally stable with a yield close to 98% after the catalyst was used seven times.

14/01829 Microalgae cultivation for bioenergy production using wastewaters from a municipal WWTP as nutritional sources

Cho, S. *et al. Bioresource Technology*, 2013, 131, 515–520.

In order to reduce input costs for microalgal cultivation, the authors investigated the feasibility of wastewater taken from a municipal wastewater treatment plant (WWTP) in Busan, Korea as wastewater nutrients. The wastewaters used in this study were the effluent from a primary settling tank (PS), the effluent from an anaerobic digestion tank (AD), the conflux of wastewaters rejected from sludge-concentrate tanks and dewatering facilities (CR), and two combined wastewaters of AD : PS (10 : 90, v/v) and AD : CR (10 : 90, v/v). *Chlorella* sp. ADE5, which was isolated from the AD, was selected for the feasibility test. The highest biomass production (3.01 g-dry cell weight per litre) of the isolate was obtained with the combined wastewater ADCR, and it was 1.72 times higher than that with BG 11 medium. Interestingly, the cells cultivated with wastewater containing PS wastewater were easily separated from the culture and improved lipid content, especially oleic acid content, in their cells.

14/01830 Multirecycling of Pu, Am and Cm in BWR

Zakova, J. and Wallenius, J. *Annals of Nuclear Energy*, 2013, 58, 255–267.

This study investigates neutronics aspects of multirecycling of Pu, Am and Cm in BWRs, employing three uranium- and three thorium-supported transmutation fuels. The results show, that thorium-based cores allow for higher shares of MA in the fuel and thereby higher MA incineration without encountering a positive total void worth at any point of the multirecycling. In the uranium-based configuration the total void worth sets the limit on the MA share around 2.45%. The thorium-based fuels also exhibit a stronger Doppler feedback and somewhat degraded reactivity as compared to uranium fuels. The alpha-heating in the fuel reaches equilibrium after six cycles, maintaining values of 24–31 W/kg^{FUEL} in the uranium-based configurations and 32–37 W/kg^{FUEL} in the thorium-based configurations. The neutron emission keeps rising through the multirecycling, the maximum value reached in the XV cycle ranges from 1.4×10^6 to 1.7×10^6 n/s/g for uranium fuels and 2×10^6 n/s/g for the thorium-based fuels.

14/01831 New hybrid absorption–compression refrigeration system based on cascade use of mid-temperature waste heat

Han, W. *et al. Applied Energy*, 2013, 106, 383–390.

This paper proposes a new hybrid absorption–compression refrigerator powered by mid-temperature waste heat. The system uses an ammonia–water binary mixture as working fluid. It consists of a heat-driven compression refrigeration subsystem and an absorption refrigeration subsystem. These refrigeration subsystems share the same condenser and evaporator. Mid-temperature waste heat is first used in the power and compression refrigeration subsystem to compress ammonia vapour from the evaporator to the condenser. Then the low-temperature waste heat is used in the absorption refrigeration subsystem to preheat the strong solution before entering the rectifier. The exhaust vapour from the ammonia–steam turbine is introduced into the rectifier of the absorption refrigeration subsystem to generate pure ammonia. The new system exhibits superior performance because of the cascade use of waste heat in the two subsystems. With the same waste heat input, the proposed system generates 46.7% more cooling energy than does a conventional ammonia–water absorption refrigerator. The system can serve as an efficient approach to producing cooling with waste heat.

14/01832 Physicochemical characterization and possible applications of the waste biomass ash from oleoresin industries of India

Abraham, R. *et al. Fuel*, 2013, 109, 366–372.

The oleoresin industries in India make use of the spice residue as boiler fuel and the combustion of this waste biomass generates tons of ash every day. This study carried out the characterization of this industrial waste ash in order to have a broad awareness of its properties in terms of toxicity, composition and possible utility. Ash collected from the grate fired furnace (bottom ash) as well the fly-ash deposited on the boiler walls and pipes were analysed. Elemental analysis of the ashes indicates its potential as a crude fertilizer or cement replacement material. PXRD indicates the presence of several crystalline phases such as harrisonite $(Ca(Fe^{3+},Mg)_6(PO_4)_2(SiO_4)_2)$, aphthitalite $((K,Na)_3Na(SO_4)_2)$, cryptomelane $(KMn_6^{4+}Mn_2^{2+}O_{16})$, varulite $(NaCaMn_{2.25}^{2+}Fe_{0.5}^{2+}Fe_{0.25}^{3+}(PO_4)_3)$, marokite $(CaMn_2O_4)$, fersilicite (FeSi) in the flyash fraction and the phases magnetite $(Fe_2^{3+}Fe^{2+}O_4)$, kalsilite $(KAlSiO_4)$, cryptomelane $(KMn_6^{4+}Mn_2^{2+}O_{16})$, fukuchilite $(Cu_3Fe^{2+}S_8)$, walthierite $(Ba_{0.5}Al_3(SO_4)_2(OH)_6)$, and magnesite $(Mg(CO_3)$ in furnace ash. The amorphous nature of silica in the ashes is evident from the characteristic broad hump around $2\theta = 30$. The iron rich fraction of the ash consists primarily of magnetite which leads to a greenish-blue colour on heating the ash above 650 °C. This magnetite fraction if separated could find use as catalysts in organic reactions. SEM images indicate the ashes to be highly agglomerated and EDX data shows the surface of the ash particles covered with potassium oxide and carbon. The percentage of K seems to be higher in the fly ash due to the volatility of the potassium compounds which is carried up by the air current. Even though the surface area of the as-received ashes is negligible, an acid treatment removes the surface adsorbed species and increases the surface area to 368 m^2/g making it an effective adsorbent.