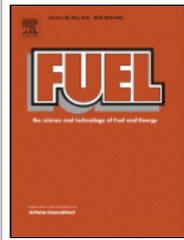


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Volume 95, Pages 1-664 (May 2012)

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Review Article

2
 Review Article
Pages 1-14
 Pasi Vainikka, Mikko Hupa
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Highlights

- ▶ Analogously to Cl, Br has a role in high temperature corrosion and dioxin formation. ▶ Bromine has natural and anthropogenic sources depending on the fuel type. ▶ Most important natural Br source is the sea. ▶ Biomass, peat and coal Br content depends on the extent of marine influence. ▶ In peat and coal Br has predominantly organic association.

Full Length Articles

3
 Original Research Article
Pages 15-18
 Tina Rita Celli Zezza, Michelle de Souza Castilho, Nelson Ramos Stradiotto
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4
 Original Research Article
Pages 19-24
 Jonathan P. Mathews, Atul Sharma
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Highlights

- ▶ The alignment of coal is quantified directly from HRTEM lattice fringe images. ▶ All coal ranks are aligned, low-rank coals to a low degree (not randomly). ▶ UF is analogous, significant contribution from fringes 90° to the alignment plane.

5
 Original Research Article
Pages 25-34
 Yuanyuan Shao, Chunbao (Charles) Xu, Jesse Zhu, Fernando Preto, Jinsheng Wang, Guy Tourigny, Chadi Badour, Hanning Li

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Highlights

► A higher chlorine content in the feed led to higher tendency of ash deposition. ► Peat pellets fuel has higher tendency of ash deposition than lignite. ► 50%Lignite–50%peat blends resulted in the lowest relative ash deposition rate. ► Moisture content of solid fuels played a positive role in reducing ash deposition. ► Adding sulfur into the fuel effectively decreased the chloride deposition.

- 6   [A molecular model for Illinois No. 6 Argonne Premium coal: Moving toward capturing the continuum structure](#) Original Research Article

Pages 35-49

Fidel Castro-Marcano, Vladislav V. Lobodin, Ryan P. Rodgers, Amy M. McKenna, Alan G. Marshall, Jonathan P. Mathews

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Highlights

► An improved computational protocol for generating coal molecular models. ► Largest, most complex coal representation constructed to-date (50,000 atoms). ► Coal model captures a portion of the continuum of structural features. ► Agrees with a wide variety of chemical and physical parameters.

- 7   [Study of *Miscanthus x giganteus* ash composition – Variation with agronomy and assessment method](#) Original Research Article

Pages 50-62

X.C. Baxter, L.I. Darvell, J.M. Jones, T. Barraclough, N.E. Yates, I. Shield

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Highlights

► We examine the impact of fertiliser and harvest time on the ash melting of *Miscanthus x giganteus*. ► Fusion temperatures of ash from leaves increase over September to March. ► Fusion temperatures in stems/whole crop ashes appear to decrease over September to March. ► Wt% K₂O in ash correlates with temperature of ash melting from the ash fusion test. ► Endotherm minimum temperature from DTA correlates with hemisphere temperature.

- 8   [Concomitant extraction of bio-oil and value added polysaccharides from *Chlorella sorokiniana* using a unique sequential hydrothermal extraction technology](#) Original Research Article

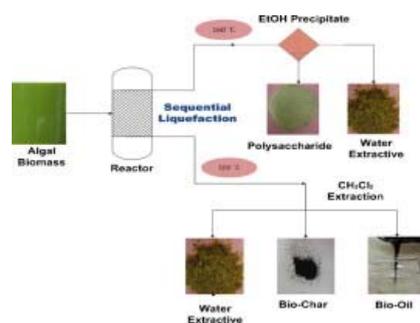
Pages 63-70

Moumita Chakraborty, Chao Miao, Armando McDonald, Shulin Chen

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Graphical abstract



Highlights

► Method uses temperature gradient for sequential extraction of desired products. ► This method successively produce polysaccharides and bio-oil from algal biomass. ► Method used, produces 63% less bio char than conventional method. ► First report of bio-oil production from heterotrophically grown *Chlorella sorokiniana*.

- 9   [Iron-based materials as tar depletion catalysts in biomass gasification: Dependency on oxygen potential](#) Original Research Article

Pages 71-78

Thomas Nordgreen, Vera Nemanova, Klas Engvall, Krister Sjöström

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Highlights

► Biomass gasification in an atmospheric fluidised bed. ► Metallic iron is used as catalyst for tar cracking. ► Oxygen potential is an important parameter for preserving the catalyst in its metallic state.

- 10  **Detailed characterization of coal-derived liquids from direct coal liquefaction on supported catalysts** Original Research Article
Pages 79-87
J. Stihle, D. Uzio, C. Lorentz, N. Charon, J. Ponthus, C. Geantet
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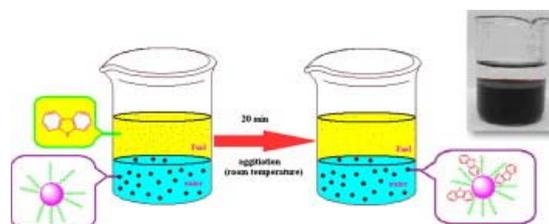
► New analytical data on a coal liquid obtained from direct coal liquefaction. ► We fractionate the coal liquid in four cuts in order to analyze them with the appropriate technique. ► GC × GC-MS and HT-GC × GC evidenced the high aromaticity of distillate and VGO cuts. ► Heteroelements are mainly in the heaviest fractions. ► The distillate cut contains high amount of normal-paraffins.

- 11  **Lipids extracted from several species of natural blue-green microalgae by dimethyl ether: Extraction yield and properties** Original Research Article
Pages 88-92
Hideki Kanda, Peng Li, Tsuyoshi Ikehara, Mina Yasumoto-Hirose
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► Lipids directly extracted from several species of high-moisture microalgae. ► The yield and molecular weight distribution is comparable to the Bligh-Dyer method. ► Extracted lipids were characterized by low O, N and higher C, H content. ► The higher calorific value of extracted lipids was 33.8 MJ/kg. ► DME extraction method also shows greater dewatering ability.

- 12  **Rapid and facile desulphurization of liquid fuel by carbon nanoparticles dispersed in aqueous phase** Original Research Article
Pages 93-96
Rahimeh Naviri Fallah, Saeid Azizian
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► Carbon nanoparticles can be prepared by a clean, cheap and convenient route. ► CNPs can be used for removal of organosulfur compounds from liquid fuel. ► This two phase system shows cheap and rapid desulfurization of liquid fuel with high efficiency.

- 13  **Investigating the rheological properties of light crude oil and the characteristics of its emulsions in order to improve pipeline flow** Original Research Article
Pages 97-107
Madjid Meriem-Benziane, Sabah A. Abdul-Wahab, Mohamed Benaicha, Mansour Belhadri
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- 14  **Microwave technology for the biodiesel production: Analytical assessments** Original Research Article
Pages 108-112
Immacolata Manco, Laura Giordani, Vittorio Vaccari, Massimo Oddone
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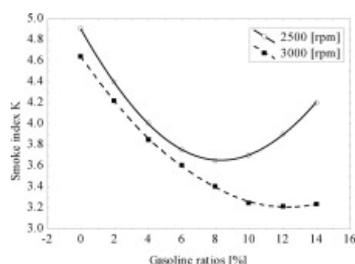
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► Biodiesel production with microwave. ► Transesterification reaction. ► Heating with pebbles.

- 15  **Experimental investigation of gasoline fumigation in a turbocharged IDI diesel engine** Original Research Article
Pages 113-121
Z. Sahin, O. Durgun, C. Bayram

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Highlights

► The amount of fumigated gasoline is adjusted by using an elementary carburetor. ► The engine operates mainly due to diesel principle. ► GF enhances the combustion process and engine efficiency increases. ► Brake specific fuel consumption, NO_x concentration and smoke index K reduces. ► GF becomes economic for this engine.

- 16  **Cold start emissions of an ethanol-fuelled engine with heated intake air and fuel** Original Research Article
Pages 122-125
Luis Carlos Monteiro Sales, José Ricardo Sodr 

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Highlights

► Heated intake air and ethanol reduces raw exhaust HC and CO emissions. ► Raw exhaust NO_x emissions are slightly reduced with heated intake air and ethanol. ► Heated intake air and ethanol increases HC and CO catalytic converter efficiency. ► NO_x catalytic reduction efficiency is unaltered by heated intake air and ethanol. ► Post-catalytic aldehydes are not altered by heated intake air and ethanol.

- 17  **Evaluation of the oxidative stability and flow properties of quaternary mixtures of vegetable oils for biodiesel production** Original Research Article
Pages 126-130
L cia M.S. Freire, Jos  R.C. Filho, Carla V.R. Moura, Luiz E.B. Soledade, Luiz Stragevitch,  ngela M.T.M. Cordeiro, Ieda M.G. Santos, Antonio G. Souza

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Highlights

► Quaternary mixtures of vegetable oils with different characteristics. ► Equilibrated composition of saturated and unsaturated fatty acids in the mixtures. ► The quaternary mixtures display better cold flow properties. ► All mixtures show better oxidative stabilities by PDSC, Petro-Oxy and Rancimat. ► Only the stability of babassu oil is better than the one of quaternary mixtures.

- 18  **Effect of oil shale retorting temperature on shale oil yield and properties** Original Research Article
Pages 131-135
Jeong Geol Na, Cheol Hyun Im, Soo Hyun Chung, Ki Bong Lee

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Highlights

► The effects of retorting temperature on the shale oil yield and properties. ► Boiling point distribution analysis was carried out. ► The retorting temperature had great effects on shale oil quality. ► Shale oil had less low-boiling point oil fraction and high-boiling point oil fraction. ► Heavy oil fractions were produced initially and light oil fractions came out later.

- 19  **Carbonyls speciation in a typical European automotive diesel engine using bioethanol/butanol-diesel blends** Original Research Article
Pages 136-145
R. Ballesteros, J.J. Hern ndez, J. Guill n-Flores

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Highlights

- Carbonyl emissions of three fuels measured along the exhaust line at four engine modes.
- Carbonyl emissions are reduced when flowing through post-treatment systems. ► Alcohol-blends emissions are higher than diesel emissions in these selected modes. ► SR got similar values in all fuels, becoming alcohol blends good diesel-substitute.

20 **Hydrolysis and glycosidation of sugars during the esterification of fast pyrolysis bio-oil** Original Research Article
Pages 146-151

Richard Gunawan, Xiang Li, Alfons Larcher, Xun Hu, Daniel Mourant, Weerawut Chaiwat, Hongwei Wu, Chun-Zhu Li

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- Hydrolysis and glycosidation of sugars during the esterification of bio-oil. ► Levoglucosan is hydrolysed and glycosidated to form methyl- α -d-glucopyranoside. ► Formation of levoglucosan from the hydrolysis of sugar oligomers. ► Temperature, catalyst loading and methanol/bio-oil ratio affect the reaction greatly.

21 **Comparison of low-field NMR and mercury intrusion porosimetry in characterizing pore size distributions of coals** Original Research Article
Pages 152-158

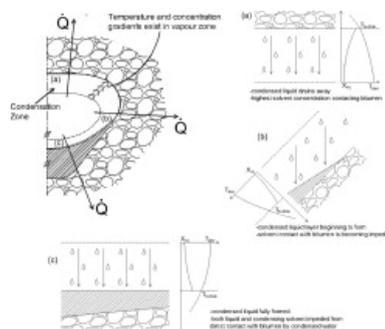
Yanbin Yao, Dameng Liu

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- NMR is compared with pressure- and rate-controlled mercury intrusion porosimetries. ► NMR is efficient for nondestructively quantifying coal pore size distribution (PSD). ► PSD determined by mercury porosimetry may inaccurate due to coal compressibility. ► PSD determined by mercury porosimetry may inaccurate due to pore-shielding-effects. ► Rate-controlled mercury porosimetry is limited to study PSD of coal macropores.

22 **Effect of vapour–liquid phase behaviour of steam–light hydrocarbon systems on steam assisted gravity drainage process for bitumen recovery** Original Research Article
Pages 159-168

Lu Dong

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- Steam–solvent phase behaviour during bitumen recovery is examined for the first time. ► Solvent only condenses first from a mixture at very high solvent concentrations. ► Water condensing first from the mixture reduces solvent contact with bitumen. ► Addition of solvent changes phase transition temperatures and enthalpies.

23 **Pyrolysis of pistachio shell: Effects of pyrolysis conditions and analysis of products** Original Research Article
Pages 169-177

Korkut Açıklalın, Fatma Karaca, Esen Bolat

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- Pistachio shell was pyrolyzed to study parameter effects on product yields. ► The most effective parameter was reaction temperature. ► Maximum liquid yield was obtained at 500 °C, 30 min and 150 ml min⁻¹ as 53.36%. ► Liquid product was a oxygenated complex mixture with 18 identified compounds. ► Solid product was a valuable fuel but wasn't suitable for active carbon applications.

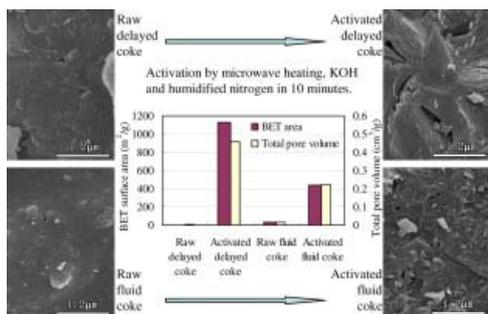
24  **Fast preparation of activated carbon from oil sands coke using microwave-assisted activation** Original Research Article

Pages 178-182
Heng Chen, Zaher Hashisho

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Graphical abstract



Highlights

► Microwaves can be used to activate oil sands coke in a short period. ► Activated coke prepared using microwave heating has high surface area and adsorption capacity. ► Microwave activation of coke can be a potential solution for the large amount of oil sands coke stockpiled in Alberta.

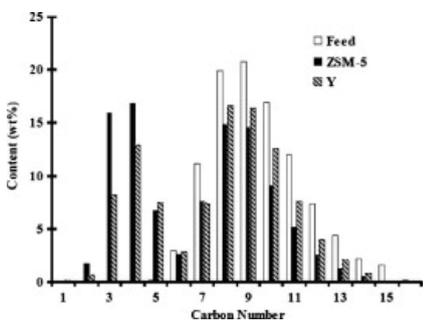
25  **Olefins production from cracking of a Fischer–Tropsch naphtha** Original Research Article

Pages 183-189
N. Fonseca, L.R.M. dos Santos, H.S. Cerqueira, F. Lemos, F. Ramôa-Ribeiro, Y.L. Lam, M.B.B. de Almeida

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Highlights

► H-ZSM-5 was more active than H-Y in the transformation of FT naphtha at 450 °C. ► Detailed PIANO analysis of the products allowed a fair estimate of the conversion. ► The transformation of the FT naphtha produces dry gas, LPG and coke. ► Products in the naphtha range were mainly naphthenics and aromatics.

26  **Estimating constituent release from FGD gypsum under different management scenarios** Original Research Article

Pages 190-196
Rachael Pasini, Harold W. Walker

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Highlights

► The LEAF methodology used to understand the leaching behavior of FGD gypsum. ► LEAF release from FGD gypsum was lower than TCLP and SPLP. ► Release from FGD gypsum in fill applications decreased with decreasing infiltration. ► Release from FGD gypsum in fill applications decreased with increasing fill depth. ► Release decreased in percolation scenarios due to saturation of pore fluid.

27  **Modelling of non-consolidated oil shale semi-coke forward combustion: Influence of carbon and calcium carbonate contents** Original Research Article

Pages 197-205
Hossein Fadaei, Mohammed Sennoune, Sylvain Salvador, Alexandre Lapene, Gerald Debenest

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Highlights

► Numerical simulation of filtration combustion in a carbon containing fixed bed. ► The model includes carbon oxidation and carbonate decomposition reactions. ► Effects of carbon and carbonate variations are studied. ► Results are confronted with the experimental work. ► A relatively simple reaction model captures the main process physics.

- 28  **Investigation of laminar flame speeds of typical syngas using laser based Bunsen method and kinetic simulation** Original Research Article
 Pages 206-213
 Yong He, Zhihua Wang, Li Yang, Ronald Whiddon, Zhongshan Li, Junhu Zhou, Kefa Cen

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Highlights

► Laminar flame speeds of typical syngas were measured by PLIF Bunsen flame. ► Kinetic simulations were validated using CHEMKIN with two mechanisms: GRI-Mech 3.0 and USC-Mech II. ► The laminar flame speed linearly increased with the increase of H₂ content.

- 29  **Evaluation of leather industry wastes as a feedstock for biodiesel production** Original Research Article
 Pages 214-220
 Ertan Alptekin, Mustafa Canakci, Huseyin Sanli

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Highlights

► The possibility of using fleshing oil in biodiesel production. ► To perform a pretreatment reaction to the fleshing oil. ► To perform the transesterification reaction, after reducing the FFA level of the fleshing oil.

- 30  **Preliminary studies on advanced power generation based on combined cycle using a single high-pressure fluidized bed boiler and consuming sugar-cane bagasse** Original Research Article
 Pages 221-225
 Marcio L. de Souza-Santos, Juan Villanueva Chavez

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Highlights

► Pressurized bubbling fluidized boiler consuming sugar-cane bagasse. ► Power generation based on steam and gas turbines. ► Simulation and optimization using comprehensive simulator (CeSFaMB former CSFMB). ► Study has already shown advantages when compared to other processes.

- 31  **Effects of initial droplet diameter and pressure on burning of ATF gel propellant droplets** Original Research Article
 Pages 226-233
 D.P. Mishra, Advitya Patyal

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Highlights

► Effects of chamber pressure and initial droplet diameter were investigated. ► Phase separation, bubble nucleation and microexplosions were observed. ► Burning rate constant increased with both chamber pressure and initial diameter. ► Higher fuel diffusion rate and reduced flame standoff ratio were the main reasons.

- 32  **Laminar burning characteristics of 2,5-dimethylfuran and iso-octane blend at elevated temperatures and pressures** Original Research Article
 Pages 234-240
 Xuesong Wu, Qianqian Li, Jin Fu, Chenglong Tang, Zuohua Huang, Ritchie Daniel, Guohong Tian, Hongming Xu

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Highlights

► Laminar flame speeds and Markstein lengths of DMF-iso-octane-air mixtures are obtained. ► Flame stabilities of the mixtures are analyzed. ► Correlation of flame speeds versus pressure and temperature are provided.

- 33  **Determination of coal ash emissivity using simplified equation for thermal design of coal-fired boilers** Original Research Article
 Pages 241-246
 Miki Shimogori, Hidehisa Yoshizako, Yukihiro Matsumura

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Highlights

► A simplified method to determine coal ash emissivity in boilers has been proposed. ► The Konopelko equation was modified based on new experimental data. ► Our method only needs iron content in ash to obtain spectral emissivity of coal ash. ► It determines total emissivities from different studies with an error of almost 20%.

34  **Effect of compression ratio on the performance and combustion of a biogas fuelled spark ignition engine**

Original Research Article

Pages 247-256

E. Porpatham, A. Ramesh, B. Nagalingam

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Highlights

► Experiments were conducted on a biogas fuelled SI engine at various equivalence ratio and number of compression ratios. ► Improvement in brake power and brake thermal efficiency with increase in compression ratio. ► Lean misfire limit is extended with increase in compression ratio. ► Enhanced compression ratio decreases hydrocarbon and carbon monoxide emission level and increase in NO emission. ► The reduction in ignition delay and higher heat release rate with increase in compression ratio.

35  **Iron oxide nanoparticles for rapid adsorption and enhanced catalytic oxidation of thermally cracked asphaltenes**

Original Research Article

Pages 257-262

Nashaat N. Nassar, Azfar Hassan, Lante Carbognani, Francisco Lopez-Linares, Pedro Pereira-Almao

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Highlights

► Fe₃O₄ nanoparticles were employed for adsorptive and oxidation of four different asphaltenes. ► The extent of adsorption increased with decrease in the molecular weight of the asphaltenes. ► Adsorption affinity increased as the molecular weight of asphaltenes increased. ► Fe₃O₄ caused a decrease in the oxidation temperature and activation energy of asphaltenes. ► Fe₃O₄ nanoparticles can serve as an excellent adsorbent/catalyst for heavy oil upgrading.

36  **Fuels from bio-oils: Bio-oil production from different residual sources, characterization and thermal conditioning**

Original Research Article

Pages 263-271

Melisa Bertero, Gabriela de la Puente, Ulises Sedran

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Highlights

► Bio-oils from the pyrolysis of various residual biomasses and their fractions were characterized. ► Bio-oil composition and physicochemical properties changed positively after thermal treatment. ► Most important changes were in phenols and heavy molecular weight compounds, CCR and EHI. ► Pine bio-oil resulted most appropriate for co-processing in FCC.

37  **Fate and abatement of mercury and other trace elements in a coal fluidised bed oxy combustion pilot plant**

Original Research Article

Pages 272-281

O. Font, P. Córdoba, C. Leiva, L.M. Romeo, I. Bolea, I. Guedea, N. Moreno, X. Querol, C. Fernandez, L.I. Díez

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Highlights

► The fate of elements and properties of ashes were evaluated in BFB coal oxy-combustion plant. ► High abatement for SO₂ and NO_x (99.9%), Hg (92.5%) and remaining elements (99.9%) is obtained. ► Low retention for Cl is achieved (19%), being the main impurity for subsequent CO₂ treatment. ► Most of the gaseous Hg occurs in the exhaust gas as Hg⁰ (81%).

38  **The optimization of low-rank coal grinding for transport coal gasification by robust design**

Original Research Article

Pages 282-286

Chong-Lyuck Park, Byoung-Gon Kim

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Highlights

► KBR transport gasifier is an effective process for gasification of low-rank coal. ► However, a feed coal for this gasifier has a narrow particle size distribution. ► Grinding parameters on hammer mill was investigated by Taguchi method. ► Aperture size of screen in the second hammer mill was the most significant factor. ► The ratio of product loss was 10.18% under the optimized condition.

39  **Atomization and vaporization for flash-boiling multi-hole sprays with alcohol fuels** Original Research Article
Pages 287-297

Wei Zeng, Min Xu, Gaoming Zhang, Yuyin Zhang, David J. Cleary

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Highlights

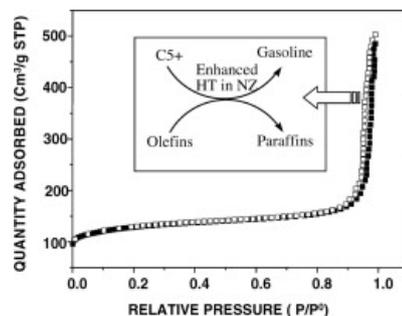
► This study used Mie-scattering and quantitative Laser Induced Exciplex Fluorescence techniques to investigate flash-boiling spray. ► The structure and vapor quantity of flash-boiling spray primarily depend on the ambient-to-saturation pressure ratio. ► The observed trends of spray structure and vapor quantity have strong inter-dependence. ► It provides correlations of spray penetration and plume width.

40  **Catalytic performance of nano crystalline H-ZSM-5 in ethanol to gasoline (ETG) reaction** Original Research Article
Pages 298-304

Nagabhatla Viswanadham, Sandeep K. Saxena, Jitendra Kumar, Peta Sreenivasulu, Devaki Nandan

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Graphical abstract**Highlights**

► The crystal size of ZSM-5 is brought down from micro to nano meter level, without affecting its acidity. ► Acid density played vital role in the formation of C₅+ oligomers, possible intermediates for gasoline formation. ► Mesopores in NZ facilitated enhanced hydrogen transfer (HT) reactions responsible for gasoline formation. ► Combination of high acid density and mesoporosity produces as high as 74 wt.% of gasoline from ethanol.

41  **Kinetic study of lignocellulosic biomass oxidative pyrolysis** Original Research Article
Pages 305-311

Maidier Amutio, Gartzen Lopez, Roberto Aguado, Maite Artetxe, Javier Bilbao, Martin Olazar

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Highlights

► This study sheds light on large-scale autothermal operation. ► The process is the sum of pyrolysis and heterogeneous oxidation and char combustion. ► The oxygen effect is significant and shifts the peaks to lower temperatures. ► The six-simultaneous-reaction model adequately fits the experimental data.

42  **Aggressiveness of a 20% bioethanol 80% gasoline mixture on autoparts: II Behavior of polymeric materials** Original Research Article
Pages 312-319

L. Baena, F. Jaramillo, J.A. Calderón

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Highlights

► Polymeric materials exposed to E20 showed mass increases below 10%. ► Ethanol absorption by some polymers is due to the high affinity of the amide group with the hydroxyl group. ► Some polymers displayed a greater hardness decrease in samples immersed in

gasoline than samples immersed in the E20. ► There were changes in the crystallinity of the PA66 after being exposed to both fuels.

- 43  **Aggressiveness of a 20% bioethanol–80% gasoline mixture on autoparts: I behavior of metallic materials and evaluation of their electrochemical properties** Original Research Article
Pages 320-328
L.M. Baena, M. Gómez, J.A. Calderón
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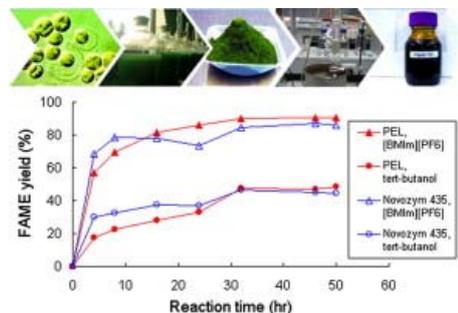
Highlights

► Carbon steel and copper exposed to E20 exhibited susceptibility to corrosion. ► Ethanolamine in the E20 mixture as a corrosion inhibitor for carbon steel was effective. ► EIS technique is useful to assess the corrosion susceptibility of metals immersed in ethanol blend fuels. ► Severe hydrodynamic conditions improve corrosion resistance of copper and tin.

- 44  **Enzymatic production of microalgal biodiesel in ionic liquid [BMIm][PF₆]** Original Research Article
Pages 329-333
Jing-Qi Lai, Zhang-Li Hu, Peng-Wei Wang, Zhen Yang
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Graphical abstract



Highlights

► Algal oil from *Chlorella* is an excellent source for biodiesel production. ► [BMIm][PF₆] is a superior solvent for enzymatic production of microalgal biodiesel. ► *Penicillium expansum* lipase (PEL) is an efficient enzyme for biodiesel production.

- 45  **Distribution and fate of environmentally sensitive elements (arsenic, mercury, stibium and selenium) in coal-fired power plants at Huainan, Anhui, China** Original Research Article
Pages 334-339
Quan Tang, Guijian Liu, Zhichao Yan, Ruoyu Sun
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Highlights

► We examine contents of As, Hg, Sb and Se in feed coals and its combustion by-products in two coal-fired power plants. ► We establish the overall material balances of these elements. ► We calculate removal efficiencies of As, Hg, Sb and Se by ESP units and FGD process. ► The total emissions of As, Hg and Se were calculated at 0.46 t, 0.04 t and 2.27 t, respectively.

- 46  **The effect of tire derived fuel/diesel fuel blends utilization on diesel engine performance and emissions** Original Research Article
Pages 340-346
Oğuzhan Doğan, M. Bahattin Çelik, Bülent Özdalyan
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Highlights

► The DI diesel engine can run by using tire derived fuel (TDF)/diesel fuel blends up to TDF90. ► Increasing TDF fraction in diesel fuel reduces the smoke, CO and HC emissions. ► Also, the NO_x emissions show increasing trend. ► The BSEC and the BTE of the TDF fuel blends are similar to diesel fuel.

- 47  **Effect of water density and air pressure on partial oxidation of bitumen in supercritical water** Original Research Article
Pages 347-351
Takafumi Sato, Phan Hieu Trung, Tomoyuki Tomita, Naotsugu Itoh
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Highlights

► Bitumen was partially oxidized in supercritical water for selective CO formation. ► The bitumen – supercritical water – air system consisted of two phases. ► The CO selectivity increased and the amount of total gas tended to decrease with increasing water/oil ratio. ► The increase in air pressure increased the amount of CO and CO₂ and decreased the CO selectivity. ► Temperature, water/oil ratio and air pressure were important factors to govern partial oxidation of bitumen.

48  **Reactive DWC leading the way to FAME and**

fortune Original Research Article

Pages 352-359

Anton Alexandru Kiss, Juan Gabriel Segovia-Hernández, Costin Sorin Bildea, Erick Yair Miranda-Galindo, Salvador Hernández

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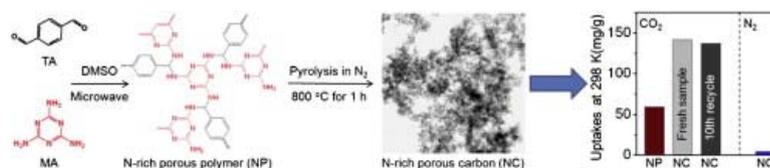
► FAME synthesis by esterification of free fatty acids (FFAs). ► Reactive distillation in a dividing wall column (DWC). ► Eco-efficient solid catalysts in high efficient equipment. ► Energy savings of 25% by optimal column design using simulated annealing. ► Rigorous simulations performed in AspenTech Aspen Plus linked to Matlab.

49  **Efficient carbon dioxide capture over a nitrogen-rich carbon**

structure Original Research Article

Pages 360-364

Chao Chen, Jun Kim, Wha-Seung Ahn

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► A new nitrogen-rich carbon having a hierarchical micro-mesopore structure was prepared. ► The effectiveness of this carbon material as a CO₂ adsorbent was evaluated. ► High CO₂ uptake and excellent CO₂/N₂ selectivity were achieved. ► CO₂ adsorption–desorption test cycles established the material's excellent stability.

50  **CCSEM investigation of respirable quartz in air samples**

activities Original Research Article

Pages 365-370

Gerald P. Huffman, Naresh Shah, Nick Cprek, Frank E. Huggins, Gary Casuccio, Everett Ramer, Jeffrey B. Hicks

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► A improved method has been developed to measure respirable quartz in coal fly ash (CFA) using computer-controlled SEM. ► CCSEM and X-ray diffraction (XRD) were used to measure respirable quartz in CFA collected at two power plants. ► CCSEM and XRD were in good agreement only for samples collected using cyclone-filtered air samplers.

51  **Characterization of tight gas reservoir pore structure using**

USANS/SANS and gas adsorption

analysis Original Research Article

Pages 371-385

C.R. Clarkson, M. Freeman, L. He, M. Agamalian, Y.B. Melnichenko, M. Mastalerz, R.M. Bustin, A.P. Radliński, T.P. Blach

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► SANS/USANS is used to characterize pore structure of a tight gas reservoir. ► The dominant pores in three tight gas samples are in the mesopore/macropore range. ► SANS/USANS-derived surface areas are higher than those derived from adsorption. ► SANS/USANS-derived porosities are higher than those derived from helium porosimetry. ► Open versus closed porosity can be determined from the combined techniques.

52 	<p>Soybean oil transesterification by the use of a microwave flow system Original Research Article <i>Pages 386-393</i> J.M. Encinar, J.F. González, G. Martínez, N. Sánchez, A. Pardal</p> <p>Show preview Related articles Related reference work articles</p>	Purchase
<p>Highlights</p> <ul style="list-style-type: none"> ▶ Biodiesel production from soybean transesterification by use of microwave flow system. ▶ We examine influences of residence time and microwave power on final temperature. ▶ Residence times between 2.5 and 14 min and microwave powers until 200 W are enough. ▶ Heating by microwave system is more effective than conventional heating. ▶ Biodiesel's properties fulfil the limits of Norm EN 14214. 		
53 	<p>Effect of functional group on thermal stability of cellulose derivative energetic polymers Original Research Article <i>Pages 394-399</i> Mojtaba Shamsipur, Seied Mahdi Pourmortazavi, Seiedeh Somayyeh Hajimirsadeghi, Seyed Mahdi Atifeh</p> <p>Show preview Related articles Related reference work articles</p>	Purchase
<p>Highlights</p> <ul style="list-style-type: none"> ▶ Thermal stability of cellulose based energetic polymers with various functional groups. ▶ Study of cellulose acetate nitrate, azidodeoxy cellulose, azidodeoxy cellulose nitrate. ▶ Elucidation of the reaction processes with simultaneous TG-DTA and DSC analyses. ▶ Stability: cellulose acetate nitrate < azidodeoxy cellulose > azidodeoxy cellulose nitrate. 		
54 	<p>Novel coal-based precursors for cokes with highly oriented microstructures Original Research Article <i>Pages 400-406</i> P. Alvarez, N. Díez, R. Santamaría, C. Blanco, R. Menéndez, M. Granda</p> <p>Show preview Related articles Related reference work articles</p>	Purchase
<p>Highlights</p> <ul style="list-style-type: none"> ▶ Novel anthracene oil pitches produce cokes with highly oriented microstructures. ▶ Less polymerized pitches required the use of pressure. ▶ Microstructure was improved by controlling reaction conditions. ▶ Less polymerized pitches led to cokes with more oriented microstructures. 		
55 	<p>Structural and rheological characterization of wax modified bitumens Original Research Article <i>Pages 407-416</i> Giovanni Polacco, Sara Filippi, Massimo Paci, Felice Giuliani, Filippo Merusi</p> <p>Show preview Related articles Related reference work articles</p>	Purchase
<p>Highlights</p> <ul style="list-style-type: none"> ▶ Synthetic hydrocarbons, natural and amidic-modified waxes as bitumen modifiers. ▶ Rheological and thermal properties of the blends related to wax chemical structure. ▶ Amidic waxes seems to establish stronger interactions with asphaltenes. ▶ In different temperature ranges, waxes differently influence blend properties. 		
56 	<p>Optimisation of particle size in waste tyre pyrolysis Original Research Article <i>Pages 417-424</i> Adetoyese Oyedun, Ka-Leung Lam, Malte Fittkau, Chi-Wai Hui</p> <p>Show preview Related articles Related reference work articles</p>	Purchase
<p>Highlights</p> <ul style="list-style-type: none"> ▶ We model the kinetics and heat flow data of waste tyre pyrolysis. ▶ Incorporation of the shredding energy into the overall energy usage. ▶ Simulation was conducted under different heating rates and heating approach. ▶ We study the effects of particle size on completion time and overall energy usage. ▶ Optimisation of particle size was conducted at different specified completion times. 		
57 	<p>Pyrolysis characteristics of sucrose biomass in a tubular reactor and a thermogravimetric analysis Original Research Article <i>Pages 425-430</i> Haisheng Chen, Binlin Dou, Yongchen Song, Yujie Xu, Yi Zhang, Chao Wang, Xuehui Zhang, Chunqing Tan</p> <p>Show preview Related articles Related reference work articles</p>	Purchase

Highlights

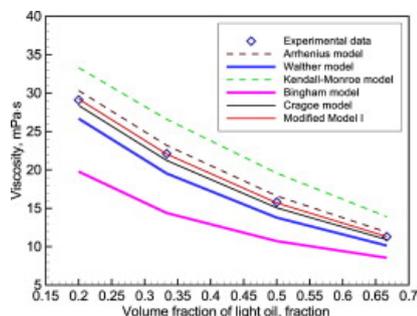
► The pyrolysis characteristics of sucrose in a tubular reactor were different from those obtained by the TG method. ► CaO greatly enhanced the rates of pyrolysis. ► The products and kinetics of sucrose pyrolysis in a tubular reactor were studied.

58  **New models for calculating the viscosity of mixed**oil
Original Research Article

Pages 431-437

Yuanping Gao, Kewen Li

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► We measure 200 viscosities of mixed oils. ► We examine five frequently-used models for calculating the viscosity of mixed oil. ► The Arrhenius model is the best of the five models. ► Our modified model I has a better accuracy than the Arrhenius model. ► Our modified model II is another kind of viscosity model.

59  **Liquid–vapor equilibria of binary systems containing alcohols (1-butanol, or 2-butanol or 1-hexanol) present in the production by chemical process of 2,5-dimethyl furan from biomass**

Original Research Article

Pages 438-445

Lamia Kara Zaitri, Latifa Negadi, Ilham Mokbel, Nizar Msakni, Jacques Jose

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► Vapor pressures of 2,5-dimethyl furan + 1-butanol, + 2-butanol or +1-hexanol. ► The investigated temperatures are 313 K and 393 K. ► (2,5-dimethyl furan + 1-hexanol) system shows maximum azeotropic behavior. ► The three binary systems exhibit positive deviations in G^E . ► The NRTL, UNIQUAC and UNIFAC models have been used.

60  **Environmental geochemistry of the feed coals and their combustion by-products from two coal-fired power plants in Xinjiang Province, Northwest China**

Original Research Article

Pages 446-456

Jing Li, Xinguo Zhuang, Xavier Querol, Oriol Font, Natalia Moreno, Jibin Zhou

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► Geochemical characteristic of feed coal and combustion by-products from power plants. ► High coal quality, low element concentrations in fly ash and low leachable potential. ► S, F, Cl, Hg, and B were highly volatile at ESP in plants. ► High amorphous glass content and SiO_2/Al_2O_3 ratio in the glass matrix of fly ash. ► High potential for a variety of uses of fly ash with low environmental limitations.

61  **A simple method for preparation of presulfided eggshell CoMoS/γ-Al₂O₃ catalysts for hydrodesulfurization of dibenzothiophene**

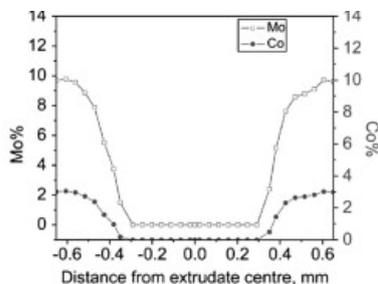
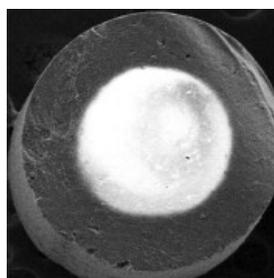
Original Research Article

Pages 457-463

Bin Liu, Yongming Chai, Yukang Liu, Yajing Wang, Yunqi Liu, Chenguang Liu

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Co and Mo distributions of the eggshell catalyst cross section

Highlights

- An effective method to prepare eggshell CoMoS/Al₂O₃ catalysts was developed.
- The eggshell thickness of Co and Mo could be easily regulated.
- The eggshell catalyst could decrease the internal diffusion limitation.
- The eggshell catalyst could improve the utilization efficiency of active components.
- The eggshell catalyst showed higher DBT HDS activity.

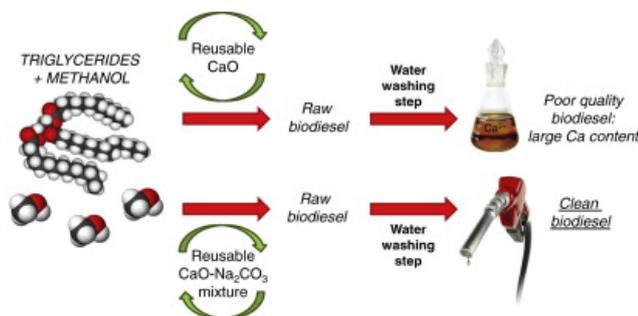
62 [A new and efficient procedure for removing calcium soaps in biodiesel obtained using CaO as a heterogeneous catalyst](#) Original Research Article
Pages 464-470

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A.C. Alba-Rubio, M.L. Alonso Castillo, M.C.G. Albuquerque, R. Mariscal, C.L. Cavalcante Jr., M. López Granados

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Highlights

- The raw biodiesel obtained by using CaO as catalyst cannot be used as biofuel.
- It contains a large concentration of Ca cations and it requires an efficient procedure to remove Ca.
- A new procedure has been developed that allows the cleansing of the raw biodiesel by a simple water washing step.
- The procedure consists of incorporating Na₂CO₃ to the initial CaO–oil–methanol reaction mixture.

63 [Multicomponent vaporization modeling of bio-oil and its mixtures with other fuels](#) Original Research Article
Pages 471-480

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Lei Zhang, Song-Chang Kong

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Highlights

- Bio-oil drop size history does not follow the conventional D²-curve due to its complex composition.
- At the end of vaporization, only levoglucosan remains in the bio-oil drop.
- Vapor distribution of bio-oil spray is consistent with the volatilities of individual components.
- The presence of bio-oil in the mixture of bio-oil and other fuels extends the drop lifetime.
- The lifetime of pure bio-oil drops is relatively longer than diesel, biodiesel, and ethanol.

64 [Molybdenum speciation in asphaltite bottom ash \(Seguruk, SE Anatolia, Turkey\)](#) Original Research Article
Pages 481-485

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Isil Aydin, Firat Aydin, Candan Hamamci

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Highlights

- There is a high level of uncertainty concerning the occurrence of molybdenum in asphaltite. This study presents the concentration and speciation of molybdenum in bottom ash of asphaltite (Seguruk, SE Anatolia, Turkey). A seven step sequential extraction process to

speciation of molybdenum from asphaltite bottom ash was investigated. The most abundant form of molybdenum in samples is sulfide fraction of molybdenum. Relative abundances of the remaining fractions follow the order:
residual > reducible > oxidizable > exchangeable > carbonate > water soluble.

65  **The impact of fuel injection pressure on the exhaust emissions of a direct injection diesel engine fueled with biodiesel–diesel fuel blends** Original Research Article
Pages 486–494

Metin Gumus, Cenk Sayin, Mustafa Canakci

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Highlights

► The influence of injection pressure on the emission characteristics of a diesel engine using biodiesel–diesel fuel blends. ► The effect of biodiesel–diesel fuel blends on the performance parameters in terms of brake specific fuel consumption. ► The possibility of using biodiesel–diesel fuel blends at different injection pressures.

66  **Study on biogas production by anaerobic digestion of garden-waste** Original Research Article
Pages 495–498

Priyanka Gupta, Raj Shekhar Singh, Ashish Sachan, Ambarish S. Vidyarthi, Asha Gupta

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Highlights

► Microbes found in cow-dung were not able to grow on garden-waste for methane production. ► Microbes present in paddy-field soil were able to grow on garden-waste. ► Microbes present in mine water were capable to utilize garden-waste as substrate to produce biogas. ► Microbes present in termite guts were able to digest garden-waste an-aerobically.

67  **Spray model based on step response theory** Original Research Article
Pages 499–503

Kesong Zhang, Zhi Wang, Jianxin Wang, Zhiming Wang

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Highlights

► Diesel spray is treated as a critical-damped second order response system. ► Spray dynamic and fluid status have been decoupled. ► Two key parameters, the density time constant and momentum time constant, are introduced.

68  **The effect of perchloroethylene on coking properties** Original Research Article
Pages 504–513

Simon M. Iveson, Kevin P. Galvin

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Highlights

► Perchloroethylene can lower fluidity and CSR and increase CRI of some coals. ► Poor coking property and high inertinite content coals were the most affected. ► Hence clean coal composites formed using heavy organic liquids may be misleading. ► Water-based laboratory methods can reliably produce clean coal composites. ► Hence these are a potential replacement for heavy organic liquid fractionation.

69  **Fast pyrolysis of a waste fraction of high impact polystyrene (HIPS) containing brominated flame retardants in a fluidized bed reactor: The effects of various Ca-based additives (CaO, Ca(OH)₂ and oyster shells) on the removal of bromine** Original Research Article
Pages 514–520

Su-Hwa Jung, Seon-Jin Kim, Joo-Sik Kim

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Highlights

► Use of a fluidized bed reactor in the pyrolysis of HIPS–Br. ► Use of a char separation system composed of a cyclone and hot filter. ► Application of various Ca-based additives including oyster shells for removal of Br.

70  **Theoretical studies of CO₂ adsorption mechanism on linkers of metal–organic frameworks** Original Research Article
Pages 521–527

Yang Liu, Jing Liu, Ming Chang, Chuguang Zheng

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Highlights

► The adsorption mechanism of CO₂ on linker of MOFs is investigated. ► The models are evaluated by comparing the adsorption energies. ► Eight different positions on linker with three orientations of CO₂ are studied. ► Chemical modifications are conducted to enhance the adsorption strength of CO₂. ► The highest adsorption energy is obtained by doping MOFs with Li atom.

- 71  **Bioethanol production from hydrothermal pretreated wheat straw by a flocculating *Saccharomyces cerevisiae* strain – Effect of process conditions** Original Research Article
Pages 528-536

Héctor A. Ruiz, Daniel P. Silva, Denise S. Ruzene, Luis F. Lima, Antônio A. Vicente, José A. Teixeira

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Highlights

► Hydrothermal processing is an efficient pretreatment for wheat straw biomass. ► *S. cerevisiae* CA11 has potential to be used for ethanol production. ► Experimental design showed the main effect onSSF processes.

- 72  **Kinetics of the gasification of a Rio Turbio coal under different pyrolysis temperatures** Original Research Article
Pages 537-543

G. De Micco, A. Nasjleti, A.E. Bohé

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Highlights

► Kinetics of gasification of Rio Turbio coal was studied by gas chromatography. ► Reactivity of the chars decrease slightly with the increase in pyrolysis temperature. ► For pyrolysis at 1223 K the CO₂ concentration has no influence in the reaction rate. ► For pyrolysis at 1123 K a 0.5 reaction order was found for CO₂ concentration below 30%. ► Reaction rate is well correlated with grain model and random pore model.

- 73  **Development of emissions predictor equations for a light-duty diesel engine using biodiesel fuel properties** Original Research Article
Pages 544-552

Jo-Han Ng, Hoon Kiat Ng, Suyin Gan

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Highlights

► Pertinent biodiesel fuel properties influencing diesel emissions were identified. ► Emission predictor equations were formulated using non-statistical graphical method. ► Basic fuel properties were found to be sufficient to predict engine-out emissions. ► Predictor equations can aid the production of designer fuels for emissions control.

- 74  **The positive effects of bed material coating on tar reduction in a dual fluidized bed gasifier** Original Research Article
Pages 553-562

Friedrich Kirnbauer, Veronika Wilk, Hannes Kitzler, Stefan Kern, Hermann Hofbauer

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Highlights

► Olivine is modified by the ash during biomass steam gasification in a dual fluidized bed system. ► A calcium rich layer is built at the surface of the bed material. ► This calcium rich layer has an influence on the product gas composition. ► This calcium rich layer reduces the tar content of the product gas for about 80%.

- 75  **Assessing the potential for biofuel production of corn stover pyrolysis using a pressurized batch reactor** Original Research Article
Pages 563-572

Jewel A. Capunitan, Sergio C. Capareda

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Highlights

► Corn stover pyrolysis yields were evaluated in a pressurized batch reactor. ► Maximum bio-char and liquid product yield were obtained at 400 °C. ► Bio-char has high heating value and composition similar to solid fuels. ► Bio-oil consisted of a wide range of chemicals based on FTIR and GC-MS analysis. ► The gas product consisted mainly of carbon dioxide, hydrogen and methane.

76  **A comparison of prairie cordgrass and switchgrass as a biomass for syngas production** Original Research Article
 Pages 573-577
 Alex Moutsoglou

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Highlights

- ▶ Gasification of switchgrass produces more H₂ and CO than prairie cordgrass does.
- ▶ Gasification of prairie cordgrass produces more CH₄ and CO₂ than switchgrass does.
- ▶ Higher H₂/CO molar ratios for gasification of switchgrass than prairie cordgrass.

77  **Diesel emissions improvements through the use of biodiesel or oxygenated blending components** Original Research Article
 Pages 578-586
 S.S. Gill, A. Tsolakis, J.M. Herreros, A.P.E. York

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Highlights

- ▶ Diglyme-ULSD blend offers a joint benefit of oxygen enrichment and cetane improvement.
- ▶ Diglyme improves the NO_x/PM trade-off of ULSD with simultaneous NO_x and PM reductions.
- ▶ Oxygenated additives can have greater potential than blending ULSD with biodiesel.

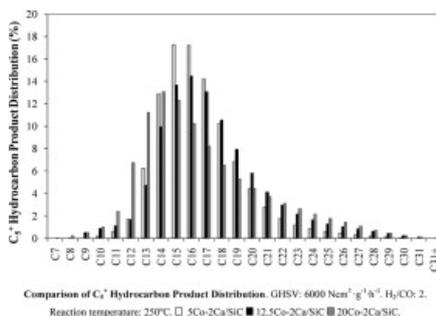
78  **Performing the best composition of supported Co/SiC catalyst for selective FTS diesel production** Original Research Article
 Pages 587-598

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Ana Raquel de la Osa, Antonio de Lucas, Luz Sánchez-Silva, Javier Díaz-Maroto, José Luis Valverde, Paula Sánchez

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Highlights

- ▶ mCo–nCa/SiC optimization for synthetic diesel bench scale Fischer–Tropsch.
- ▶ Response surface methodology to evaluate basicity, particle size and reduction.
- ▶ Only reduction shows non-linear dependence on Co, with a maximum at 14 wt.%.
- ▶ Basicity and degree of reduction clearly modify selectivity and CO conversion.
- ▶ A composition of 12.5 wt.% Co with 2.0 wt.% Ca provided the maximum diesel yield.

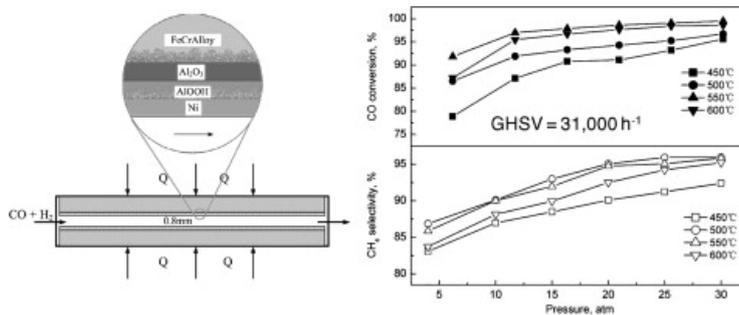
79  **Total methanation of syngas to synthetic natural gas over Ni catalyst in a micro-channel reactor** Original Research Article
 Pages 599-605

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Zhihong Liu, Bozhao Chu, Xuli Zhai, Yong Jin, Yi Cheng

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Graphical abstract



Highlights

► Novel (micro-)channel reactor for methanation reaction from syngas to SNG. ► Metal-ceramics complex substrate: superior heat conduction and firm catalyst coating. ► Excellent reactor performance at 450–550 °C and 30 atm. ► Highly efficient reactor design with milliseconds contact time (e.g., 70,000 h⁻¹).

80  **Ethanol production from poplar wood through enzymatic saccharification and fermentation by dilute acid and SPORL pretreatments** Original Research Article

Pages 606-614

Z.J. Wang, J.Y. Zhu, Ronald S. Zalesny Jr., K.F. Chen

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Highlights

► Evaluate the bioconversion potential of four poplar wood samples to sugar and ethanol. ► Found lignin affecting bioconversion the poplars through protecting carbohydrate degradation. ► SPORL improved bioconversion of all wood samples and tolerance to feedstock variability.

81  **Air and noise pollution of a diesel engine fueled with olive pomace oil methyl ester and petrodiesel blends** Original Research Article

Pages 615-621

M.D. Redel-Macías, S. Pinzi, D. Leiva, A.J. Cubero-Atienza, M.P. Dorado

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Highlights

► We proposed the use of low quality olive pomace oil to produce biodiesel. ► Cetane number depicts a stronger influence over noise production than bulk modulus. ► Bulk modulus exhibits a stronger influence over NO_x emissions than cetane number. ► Biodiesel blends reduce air and noise pollution and improve sound quality.

82  **Hydrocarbon fuels from vegetable oils via hydrolysis and thermo-catalytic decarboxylation** Original Research Article

Pages 622-629

Wei-Cheng Wang, Nirajan Thapaliya, Andrew Campos, Larry F. Stikeleather, William L. Roberts

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Highlights

► Converting vegetable oil into hydrocarbon fuel using hydrolysis and decarboxylation. ► The free fatty acid conversion from hydrolysis has yielded at 99.7%. ► The decarboxylation average rate was determined as 15.5 mmoles/min. ► The cold flow properties of the fuel was improved using isomerization process.

83  **Microwave-assisted extraction of Xianfeng lignite in 1-butyl-3-methyl-imidazolium chloride** Original Research Article

Pages 630-633

Zhiping Lei, Lian Wu, Yanqiu Zhang, Hengfu Shui, Zhicai Wang, Chunxiu Pan, Haiping Li, Shibiao Ren, Shigang Kang

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Highlights

► [Bmim]Cl has high performance on the extraction of lignite. ► Effect of temperature and ratio of lignite/[Bmim]Cl on the lignite extract yield. ► [Bmim]Cl breaks hydrogen bonds in lignite and extracts the aromatics from lignite.

84  **Characterization of model compounds of processed lignin and the lignome by using atmospheric pressure ionization tandem mass spectrometry** Original Research Article

Pages 634-641

Laura J. Hauptert, Benjamin C. Owen, Christopher L. Marcum, Tiffany M. Jarrell, Christopher J. Pulliam, Lucas M. Amundson, Padmaja Narra, Mohammad Sabir Aqueel, Trenton H. Parsell, Mahdi M. Abu-Omar, Hillka I. Kenttämä

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Highlights

► Negative ion mass spectrometry for the characterization of degraded lignin. ► (-) ESI with NaOH dopant ionizes lignin model compounds without fragmentation in MS. ► CAD MS/MS yields structural information for deprotonated lignin model compounds.

85  **The effect of additives on coking pressure and coke quality** Original Research Article

Pages 642-647

A.M. Fernández, C. Barriocanal, R. Alvarez

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<p>Highlights</p> <p>► We studied the possibility of reducing coking pressure by means of additives. ► The most effective additive for reducing coking pressure is coke fines. ► A low volatile PCI coal is more effective than a high volatile PCI coal as coking pressure reducer. ► The cokes that contain coke fines present very low CSR values. ► The low volatile matter PCI coal is the best additive for reducing coking pressure without impairing coke quality.</p>		
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<p>Highlights</p> <p>► Three RE–W electrostatic precipitation cathodes were prepared. ► RE–W cathode electron emission properties were examined and analyzed. ► Y–W cathode shows the best emission properties at atmosphere pressure. ► Collection performance of a high temperature Y–W cathode ESP was investigated. ► Higher resistivity particles tend to be collected effectively at high temperature.</p>		
<p>Short Communications</p>		
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<p>Highlights</p> <p>► Determination of the acid number of biodiesel. ► Acid–base titration. ► Green method. ► Ethanol and water used as solvents. ► Applied to biodiesels from soy, corn, canola, castor and sunflower oils and from swine lard.</p>		
89	<p> Dry matter losses in combination with gaseous emissions during the storage of forest residues Pages 662-664 Xiao He, Anthony K. Lau, Shahab Sokhansanj, C. Jim Lim, Xiaotao T. Bi, Staffan Melin</p> <p>Show preview Related articles Related reference work articles</p>	<p>Purchase</p>
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