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THE SHORTENING OF LIFT-OFF LENGTH ASSOCIATED WITH JET-WALL AND JET-JET INTERACTION IN A SMALL-BORE OPTICAL DIESEL ENGINE

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ABSTRACT

Jet-wall and jet-jet interactions are important diesel combustion phenomena that impact fuel-air mixing, flame lift-off and pollutant formation. Previous studies to visualise a wall-interacting jet in heavy-duty diesel engines suggested that the shortening of lift-off length could occur due to the recirculated hot combustion products that are entrained back into incoming diesel jet. The significance of this effect, known as re-entrainment, can be higher in small-bore engines due to shorter nozzle-to-wall distance and increased wall curvature. In this study, we performed hydroxyl chemiluminescence imaging using an intensified CCD camera and high-speed imaging of natural soot luminosity using a CMOS camera in an automotive-size optical diesel engine. To provide detailed understanding of the reacting jet under the influence of re-entrainment as well as jet-jet interaction, various jet trajectories were investigated using one and two-hole injectors coupled with a modified piston that allows (1) the identification of the shortening of lift-off length, (2) the measurements of lift-off lengths for varying degrees of jet-wall interactions and (3) the clarification on inter-jet spacing effects on the lift-off lengths. Findings from the measurements support the re-entrainment theory because the shortening of lift-off length occurs only before the end of injection when the strong jet momentum induces the ambient gas entrainment. The shortening also shows good correspondence with the penetration of the recirculated jet head back towards the centre of the combustion chamber. Simultaneous imaging of the bowl-wall-interacting jet and cylinder-liner-wall-interacting jet depicts a shorter lift-off length for the bowl-wall-interacting jet, which further supports the importance of re-entrainment on diesel combustion. Inter-jet spacing effects on the lift-off length are also studied utilising two-hole injectors with two inter-jet spacing angles (51.4° and 102.8°). A narrower spacing between the jets results in the shorter lift-off length of the primary jet due to the higher jet-jet interaction even if short injection duration is used to suppress the re-entrainment. For tested conditions of this study, the shortening of lift-off length appears to be more sensitive to jet-jet interaction than to the re-entrainment caused by the jet-wall interaction.

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EFFECT OF PARTICLE SIZE ON THE COMPOSITION OF LIGNIN DERIVED OLIGOMERS OBTAINED BY FAST PYROLYSIS OF BEECH WOOD

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ABSTRACT

The effect of particle size on the yield and composition of lignin derived oligomers (also known as pyrolytic lignin (PL)) was studied in a fluidized bed reactor. Milled beech wood particles of sizes between 0.3 and 0.55 and cylinders of 3–14 mm were pyrolyzed at 500 °C. The lignin oligomers were isolated from bio-oil and analyzed using several analytical techniques (TG, Py-GC/MS, and ¹H NMR). The yield of PL fraction decreased half when particle size raised from 0.3 to 3 mm. DTG analysis of the PL showed higher loss rates between 200 and 600 °C as particle size increased from 0.55 to 3–4 mm. Py-GC/MS results suggested a dramatic decrease of methoxylated phenols (in line with the ¹H NMR studies) and the loss of ether bonds when the particle size was increased from milled small particles of 0.3 mm to cylinders with a diameter between 3 and 5 mm. In general, most chemical changes and changes in PL yield occur between the milled particles (composed mainly of the cell wall) and cylinders with original wood structure. Comparing the milled particles to the cylinders with equal length (equal vapor outflow distance) but varied diameter, the effect on the yield of PL seems to be mainly due to the impact of thermally ejected oligomers on internal cell walls of biomass particles (mass transfer limitations).

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TRANSIENT MEASURING METHOD FOR INJECTION RATE OF EACH NOZZLE HOLE BASED ON SPRAY MOMENTUM FLUX

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ABSTRACT

For a diesel engine equipped with multi-hole injectors, its combustion process, pollutant formation and thermal load consistency of combustion chamber are directly influenced by the differences in injection rates among nozzle holes. However, there are few measuring methods and equipments suitable for the determination of injection rate of each nozzle hole. The aim of this paper is to evaluate a measuring method proposed based on the spray momentum measurement of each nozzle hole that could be used to determine its injection rate. For this purpose, a conventional injection system of pump-line-nozzle was utilized and a dedicated experimental rig was constructed. Under different operating conditions, the cycle fuel injection quantities of the measured injector and the transient injection rate of each nozzle hole were measured successively. Based on the experimental results, the reliability and stability of the proposed measuring method were validated, and the differences in injection rates among nozzle holes were analyzed. In order to further understand the measuring method proposed, the influence of the measurement procedure details such as the distance between the outlet and the target and the angle between the target and spray axis on the determination of the transient injection rate of each nozzle hole was experimentally studied. The experimental results show that when the distance between the outlet and the target is less than 12 mm and the angle between the target and spray axis is lower than 100° , the transient injection rate of each nozzle hole could be measured accurately using the measuring method proposed, and that with a higher injection pump speed or more cycle fuel supply quantity, the consistency of cycle fuel injection quantities among nozzle holes is improved gradually. The further increase of the distance or the angle will result in the reduction of the peak injection rate and cycle fuel injection quantity of the measured nozzle hole. Besides, the injection start, injection end, and the corresponding phase of peak injection rate of the measured nozzle hole will be delayed little by little with the further increment of the distance.

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EFFECTS OF DIFFERENT MEDIATORS ON ELECTRICITY GENERATION AND MICROBIAL STRUCTURE OF A TOLUENE POWERED MICROBIAL FUEL CELL

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ABSTRACT

Neutral red and potassium ferricyanide are two electron mediators that can increase the efficiency of microbial fuel cells (MFCs) via significantly different mechanisms. In this study, effects of the two mediators on electricity generation and microbial structure of a toluene powered MFC was first investigated. The maximum voltage (V_{max}) was 110.4 mV and the half-saturation constant (K_s) was 12.8 mg/L in the absence of mediators. Although the power generation efficiency was increased when adding modest amount of mediators to the anode, the toluene degradation time was 1.56–2.15 times longer than that of unmediated MFC's, relying on the mediator used. Denaturing gradient gel electrophoresis (DGGE) analysis showed a mediator-related characteristic of the microbial structure in the MFC. Results of this investigation can be used as a basis for future assessment and design of MFCs powered by xenobiotics-contaminated wastewater, such as toluene.

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ENGINE PERFORMANCE AND EMISSION CHARACTERISTICS OF HYDROTREATED VEGETABLE OIL IN LIGHT DUTY DIESEL ENGINES

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ABSTRACT

Biodiesel, of which typical material is known as FAME (Fatty Acid Methyl Ester), has some demerits such as high density and low caloric value despite better reduction on emission and lubricity when compared to petro-diesel (petroleum-derived diesel). Iso-HVO (isomerized-hydrotreated biodiesel), on the other hand, has strong competitive advantages that overcome such weak points of conventional biodiesel. The study of engine performance was carried out to compare iso-HVO with BD (Biodiesel). The **test** samples were prepared 16 kinds of fuels, which are petro-diesel and 2%, 10%, 20%, 30%, 50% of BD, HVO, and iso-HVO blended diesel, respectively. The engine performances and emission were tested on engine dynamometer and chassis dynamometer with 1.5 l diesel engine and passenger car, for evaluating maximum power, fuel consumption, and emission, especially PM (Particulate Matter) and NO_x. Iso-HVO has much better engine performance than BD and slightly better than HVO, but slightly worse than petro-diesel. On the emission, iso-HVO and HVO blended diesel emit less THC and CO than BD, even though iso-HVO blended diesel emits similar level of NO_x and PM to BD blended. All three kinds of 50% blended biofuels showed that the decrease of particle concentrations at all size range than petro-diesel.

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EXPERIMENTAL INVESTIGATION OF THE EFFECT OF ANTIOXIDANT ADDITIVES ON NOX EMISSIONS OF A DIESEL ENGINE USING BIODIESEL

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ABSTRACT

In this study, the effect of the antioxidant additives on the oxidation stability of biodiesel and the exhaust emissions of a diesel engine has been studied. Biodiesel used in this study was produced via transesterification process from canola oil, and was blended with diesel fuel 20% by volume (B20). Antioxidant additives butylated hydroxyanisole (BHA), butylated hydroxytoluene (BHT), *tert*-butylhydroquinone (TBHQ) and 2-ethylhexyl nitrate (EHN) were individually dissolved at concentrations of 0, 500, 750 and 1000 ppm by weight in B20 fuel blend for experiments. The test results of oxidation stability showed that the effectiveness of the antioxidants was in the order of TBHQ > BHA > BHT > EHN. According to exhaust emissions test results, antioxidant additives had quite effects on oxides of nitrogen (NO_x), carbon monoxide (CO) and hydrocarbon (HC) emissions of diesel engine running on biodiesel. A 1000 ppm concentration of EHN additive was optimal as NO_x levels were substantially reduced in the whole engine speed in comparison with B20 fuel.

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INEXPENSIVE CALCIUM-MODIFIED POTASSIUM CARBONATE SORBENT FOR CO₂ CAPTURE FROM FLUE GAS: IMPROVED SO₂ RESISTANCE, ENHANCED CAPACITY AND STABILITY

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ABSTRACT

Many sorbents have been studied for their CO₂ sorption capacities with CO₂ and N₂ mixture. In reality, flue gases contain SO₂. This **research** was designed to develop and evaluate an inexpensive and robust CO₂ sorbent for actual flue gas. Ca(OH)₂, CaO and CaCO₃ were explored to serve as additives of K₂CO₃/γ-Al₂O₃ for CO₂ capture. The three additives were characterized using different methods including thermal gravimetric, X-ray diffraction analyses and so on. It was found that Ca(OH)₂ is the best additive of K₂CO₃/γ-Al₂O₃ for CO₂ capture. The performances of K₂CO₃/Ca(OH)₂/γ-Al₂O₃ were evaluated with a fluidized bed reactor under different conditions including the presence of SO₂. Experimental results show that **introduction** of Ca(OH)₂ made K₂CO₃/Ca(OH)₂/γ-Al₂O₃ not only **more** capable in adsorbing CO₂ but also more robust within SO₂-containing flue gas. Thus the research work provides useful information for further development and subsequent commercialization of K₂CO₃/Ca(OH)₂/γ-Al₂O₃ in coal-fired power plants.

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EVALUATION OF OPTIMAL ACTIVITY COEFFICIENT MODELS FOR MODELING AND SIMULATION OF LIQUID-LIQUID EQUILIBRIUM OF BIODIESEL + GLYCEROL + ALCOHOL SYSTEMS

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ABSTRACT

Biodiesel is considered a good alternative for diesel engines, given its characteristics, for being non-toxic and for being a more environmental-friendly fuel. A liquid-liquid equilibrium (LLE), comprising biodiesel + glycerol + alcohol, occurs during the production of biodiesel. The use of reliable thermodynamics models is essential to describe biodiesel + glycerol + alcohol systems as to design and analyze the process and its equipment. In this work, experimental data of 34 different systems (27 for biodiesel + glycerol + alcohol; and 7 for methyl oleate + glycerol + methanol) were used for parameter estimation and to evaluate four of the main activity coefficient models (ASOG, UNIFAC, UNIFAC-LLE and UNIFAC-Dortmund) that could be used with biodiesel systems. Additionally, binary parameters for glycerol/methanol, methanol/methyl oleate and glycerol/methyl oleate have been estimated by NRTL and UNIQUAC models. Root mean square deviations (RMSD) have been used to compare experimental and simulated data. RMSD analysis showed that the UNIFAC-Dortmund model was the model that best represented the biodiesel liquid-liquid equilibrium. Best representation of the system followed the order: UNIFAC-Dortmund > ASOG > UNIFAC-LLE > UNIFAC > UNIQUAC > NRTL.

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THE RELATIONSHIP BETWEEN SPECIATION AND RELEASE ABILITY OF MERCURY IN FLUE GAS DESULFURIZATION (FGD) GYPSUM

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ABSTRACT

Multipurpose utilization of flue gas desulfurization (FGD) gypsums releases mercury into environment and poses threats to public health. Determining Hg speciation is essential not only for predicting its toxicity and mobility but also for designing effective remediation strategies. Sequential chemical extraction (SCE) method was used to analyze Hg speciation in this study. The total Hg concentration in four samples ranged from 0.61 to 1.63 $\mu\text{g/g}$. XRD and EDX analysis revealed that the main chemical composition of FGD gypsum was calcium sulfate (CaSO_4). SCE result indicated that Hg was mainly distributed in the strong complex phase, ranging from 60% to 80%. Water soluble mercury in Sample SX accounted for 30% of the total extract, which might be attributed to the relatively high chlorine content in coal. Moreover, the mobility of Hg from FGD gypsum was also investigated in this study, which exhibited biphasic kinetics. The rapid release of Hg was related to the ratio of water soluble Hg at some extent ($R^2 = 0.818$), which signified of more attentions for its stabilization. This study also suggested theoretical framework for the environmental risk associated with FGD gypsum during its usage and disposal.

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PARTITIONING OF ELEMENTS FROM COAL BY DIFFERENT SOLVENTS EXTRACTION

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ABSTRACT

Mixed samples of the whole seam and coal ply sample #1, 3, 9, 10, 14, 19, and 23 of the No. 11 coal seam from the Antaibao mining district, Shanxi, China were conducted by the sequential chemical, carbon disulfide/N-methyl-2-pyrrolidone (CS₂/NMP) mixed solvent, and fractional (methanol, benzene, acetone and tetrahydrofuran (THF)) extraction experiments. More than 30 major and trace elements in the coal samples and resultant extracts were determined by means of instrumental neutron activation analysis (INAA), inductively coupled plasma atomic emission spectroscopy (ICP-AES), inductively coupled plasma mass spectroscopy (ICP-MS) and atomic fluorescence spectrometry (AFS) in order to investigate their partitioning during the extraction. The results show that: (1) generally, an element with a higher content in coal is relatively enriched in organic solvent extracts of the coal, though its content in the extracts is significantly lower than that in the original coal. However, some elements occurring as organic phase like Br, Mo, Ni, Sb and Se are relatively enriched in the extracts; (2) the contents of most studied elements in different organic solvent extracts of coal are positively correlated with the polarity of solvent, i.e. most elements have the highest content in the methanol extract, higher in the acetone and THF extracts, and the lowest in the benzene extract in the order of the solvent polarity; (3) most studied elements have the highest extraction rate by sequential chemical extraction, higher by CS₂/NMP mixed solvent extraction, and the lowest by fractional extraction. The difference in extraction rate could reflect the affinity of elements with small or large organic molecules in coal. In detail, elements Al, As, Co, Cr, Ni, and Zn more enriched in the fractional extracts have a higher affinity with small molecules, while the other studied elements are more related to larger molecules.

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EXHAUST EMISSIONS PROGNOSTICATION FOR DI DIESEL GROUP-HOLE INJECTORS USING A SUPERVISED ARTIFICIAL NEURAL NETWORK APPROACH

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ABSTRACT

Broad information on exhaust emissions facilitates the design of modern machinery and processing equipment with modified quality specifications. This paper is aimed at investigating soot and NO_x emissions as affected by crank-angle, liquid mass evaporated, mean diesel mass fraction and heat release rate of group-hole injectors utilizing computational fluid dynamics (CFD) while the objective parameters are prognosticated by a supervised artificial neural network (ANN). A feed-forward ANN with standard back propagation (BP) learning algorithm was adopted for problem modeling with varying number of neurons in the hidden layer. A 4-17-2 topology with Levenberg–Marquardt training algorithm (trainlm) denoted mean squared error (MSE) and mean relative error (MRE) of 0.8051 and 0.0818, respectively. The supervised ANN also represented coefficient of determination, R^2 of 0.9716 and 0.9678 for NO_x and soot emissions, respectively. The obtained results have shed light on promising ability of ANN as a powerful modeling tool for prognostication of soot and NO_x emissions due to some spray specifications.

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EFFECTS OF TEMPERATURE ON THE PHYSICOCHEMICAL CHARACTERISTICS OF FAST PYROLYSIS BIO-CHARS DERIVED FROM CANADIAN WASTE BIOMASS

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ABSTRACT

Bio-chars are produced by means of a mobile pyrolysis unit from fast pyrolysis of different types of Canadian waste biomass including agricultural waste (wheat straw and flax straw), forest residue (sawdust) and animal manure (poultry litter). They were analyzed for their physicochemical changes with pyrolysis temperature (400–550 °C). To study the chemical nature of bio-char samples, analyses such as XRD, FTIR, Raman spectroscopy, XPS, SEM, ICP, TGA and electrical conductivity measurements were performed. ICP-MS analysis showed that poultry litter-derived bio-char had the largest concentration of inorganic elements (~200,000 ppm) followed by wheat straw, flax straw and sawdust derived bio-chars. In addition, the alkaline elements were 4–14 times that of essential elements (Fe and P) and 18–57 times that of heavy elements. Electrical conductivity of bio-chars, a measure of their salinity, was maximum for all samples prepared at 400 °C. SEM showed that sawdust derived bio-chars retained relatively less dissociated surfaces compared with other bio-chars. XRD confirmed the presence of sylvite, dolomite and quartz in the bio-chars. The deconvoluted XPS spectra indicated that for all precursors except poultry litter, aromatic/aliphatic carbon portion increased in the corresponding bio-char with the pyrolysis temperature. For all precursors, O/C mass ratio decreased with an increase in the pyrolysis temperature due to the development of compact aromatic structure in bio-char. This result was confirmed by a drastic increase in I_D/I_G (defect to graphitic carbon) ratio of bio-char samples produced at 550 °C from the deconvolution results of Raman spectroscopy. Thermogravimetric analysis showed that biomass decomposition started at lower temperatures for the following order: poultry litter, wheat straw, flax straw and sawdust.

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INVESTIGATION OF THE SPONTANEOUS COMBUSTION
SUSCEPTIBILITY OF COAL USING THE PULSE FLOW CALORIMETRIC
METHOD: 25 YEARS OF EXPERIENCE

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ABSTRACT

The paper summarises 25 years of experience with pulse flow calorimetry (PFC) as a method to assess the potential of coals to spontaneously heat up using the values of oxidation heat q^{30} (W kg^{-1}). During the period, about 300 coals of various rank and with natural moisture content were investigated, the maximum propensity to oxidation being found in subbituminous coals with moisture content of about 20%. The highest value of oxidation heat q^{30} was found to be 10.5 W kg^{-1} . Oxidatively altered bituminous coals are presented as coals of evidently increased ability to oxidize, and the reasons for the increased oxyreactivity are reported. Limiting values of q^{30} heat are then given to rank the coals according to the categories of self-heating risk. Finally, a comparison between oxidation heat q^{30} and the values of the initial rate of heating (IRH) of adiabatic oxidation tests is presented.

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A FULLY COUPLED HYDRO-THERMO-MECHANICAL MODEL FOR THE SPONTANEOUS COMBUSTION OF UNDERGROUND COAL SEAMS

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ABSTRACT

The spontaneous combustion of underground coal seams involves complex interactions between geomechanical effects, oxygen transport and flow, and energy transport in the porous coal media. Prior studies normally ignore the thermo-mechanical effects such as gas and coal expansion due to the self-heating of coal, and have not implemented these complex interactions fully into their simulations. In this study, a fully coupled model of coal mechanical deformation, gas flow and transport, and heat transport is developed and their complex interactions are defined through a suite of coal property models and equation-of-states. These include (1) coal porosity model; (2) coal permeability model; (3) gas equation-of-state; and (4) self-heating model.

Applying the model to quantitatively predict the time and locations of spontaneous combustion of underground gob-side entry in the Dongtan coal mine, the results are in good agreement with the in situ measurements. Besides, a significant self-accelerating-heating effect induced by the gas thermal expansion and subsequent gas pressure gradient increase is found in the self-healing process of coal through the comparison results from our model with other models. Furthermore, the self-heating susceptibilities of gob-side entry associated with extrinsic and intrinsic factors, incorporating coal permeability, pressure difference, oxygen-consumption rate, and reaction heat of coal oxidation, are gained insight using the verified model, which suggests the self-heating rate and gas velocity are positively correlated with above factors showing “S-type” upward trends, whereas the oxygen concentration has an “S-type” downward trend. The simulated results can provide some suggestions as to how to control the variables or parameters to retard or suppress the spontaneous combustion of porous coal media.

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INVESTIGATING THE RELATIVE CONTRIBUTION OF OPERATIONAL PARAMETERS ON PERFORMANCE AND EMISSIONS OF A COMMON-RAIL DIESEL ENGINE USING NEURAL NETWORK

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ABSTRACT

Engine performance and emissions depend on a variety of parameters affecting the engine. Thanks to utilization of modern diesel engine with mechatronic systems, the number engine actuators increase significantly. The actuators can affect the internal states (operational parameters) of diesel engine such as inlet manifold pressure, EGR rate, quantity and timing of pilot and main injection which in turn will influence the engine emissions and performance. These internal states can be considered as boundary conditions of in-cylinder combustion process. Due to large number of effective parameters, study of relative contribution of these states on engine outputs will be helpful in better controlling and calibration of diesel engines. In this paper, comparative effects of internal states on both performance and emissions are investigated using statistical method and ranked based on their importance. Ten engine operational parameters including: injected fuel mass, pilot and main injection mass, main and pilot injection timing, inlet air pressure and temperature, exhaust pressure, fuel rail pressure and exhaust gas recirculation rate (EGR) are considered and their influence on brake torque, Soot, NO_x and brake specific fuel consumption (BSFC) is investigated. A thermodynamic model of engine cycle is developed in AVL Boost®; the model is tuned and validated using experimental data. In order to better and faster study the effects of operational parameters on engine performance, a neural network is employed. The required data to train the neural networks is provided by using AVL Boost Design Explorer. Due to large number of inputs and outputs, a low-discrepancy and low-dispersion sequences generator called Sobol method is used to generate quasi random sequences of input data. More than 4000 engine operation points are generated and simulated in AVL Boost. The provided data is then used to train a feed forward neural network using Bayesian training method. Comparison between experimental data and simulated results shows about 6% error in prediction of the outputs. The engine performance and emission is then analyzed using both graphical and statistical methods to study how different input parameters can influence the engine emissions and performance. Finally, the relative importance of each parameter on different engine performance and emission characteristics are investigated using perturbation method and most influential parameters on different outputs are obtained

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EFFECTIVENESS OF COMO AND NIMO CATALYSTS ON CO-HYDROPROCESSING OF HEAVY ATMOSPHERIC GAS OIL-WASTE COOKING OIL MIXTURES

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ABSTRACT

Co-hydroprocessing of fossil fractions with lipids is an alternative pathway for integrating biomass in the transportation sector. This work involves the evaluation of two commercial hydrodesulfurization (HDS) catalysts in terms of their effectiveness and suitability for hydroconversion of heavy atmospheric gas oil (HAGO) and waste cooking oil (WCO) mixtures. As the most common catalysts for conventional gas oil hydroprocessing are CoMo and NiMo over Al_2O_3 , this work focused on comparing a CoMo/ Al_2O_3 and a NiMo/ Al_2O_3 catalyst with respect to the resulting diesel selectivity and quality. Both catalysts were investigated for three feedstocks including pure HAGO, a low WCO content (10% v/v) HAGO/WCO and a higher WCO content (30% v/v) HAGO/WCO mixture under three different reactor temperatures (330 °C, 350 °C and 370 °C). All the experiments were performed at constant pressure 812 psig, liquid hourly space velocity (LHSV) 1 h^{-1} and H_2/Oil ratio 505.9 nl/l. The results have shown that the catalyst HDS efficiency depends primarily upon the reaction temperature and HAGO to WCO ratio, but is quite different for both catalyst types. The HDS effectiveness of the NiMo catalyst is not affected by the addition of WCO, even in the lowest temperature (330 °C), while the one of the CoMo catalyst is strongly affected by WCO. The presence of WCO in the feedstock was proven favorable for both diesel yield and saturation, for both catalysts, but affected strongly the deactivation rate of the CoMo catalyst. Based on the experimental results obtained via this study, it was evident that NiMo type catalysts are more suitable for co-hydroprocessing of petroleum fractions with lipid containing feedstocks.

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GRAVITY DISCHARGE CHARACTERISTICS OF BIOMASS-COAL BLENDS IN A HOPPER

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ABSTRACT

Adding biomass particles into pulverized coal may significantly improve the flowability of the cohesive pulverized coal particles. Experimental study of solids discharge flow from a cylindrical hopper with no aeration revealed an interesting “needle particle effect”, which was believed to be responsible for the smoother solids discharge and significantly increased discharge rates of the coal-biomass blends within the limits of the study. The mechanisms behind the needle particle effect in a gravity discharge system, including adherence, lowering cohesion, arch-breaking and transition of flow pattern, are analyzed and verified by the experimental results. The blends behaved different when different types of biomass particles were added. The observed flowability of the blends was strongly affected by the aspect ratio and surface roughness of the biomass particles. A revised model based on Crewdson’s equation is proposed to predict the gravity discharge rate of biomass-coal blends.

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HIGH PRESSURE PHYSICOCHEMICAL PROPERTIES OF BIODIESEL COMPONENTS DERIVED FROM COCONUT OIL OR BABASSU OIL

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ABSTRACT

The four main components of biodiesel coming from coconut oil or babassu oil studied in this work are methyl caprylate, methyl caprate, methyl laurate, and methyl myristate. The speeds of sound in methyl caprylate, methyl caprate, methyl laurate were measured at pressures up to 101 MPa within the temperatures from 293 to 318 K and in methyl myristate at pressures up to 91 MPa and at temperatures from 298 to 318 K. The densities were measured under atmospheric pressure in the temperature range from 273 to 363 K for methyl caprylate, methyl caprate, between 283.15 and 363.15 K for methyl laurate and at temperatures from 293.15 to 363.15 K for methyl myristate. The densities, isobaric thermal expansivities, and isentropic compressibilities as a function of temperature and pressure have been calculated using the experimental results. The results obtained show that for a given temperature, the differences between densities of the methyl caprylate, methyl caprate, methyl laurate, and methyl myristate increase with increasing pressure, while for a given pressure the differences between densities of the methyl esters under test decrease with increasing temperature, which leads to cross of density isobars.

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INFLUENCE OF OVEN CONFIGURATION

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ABSTRACT

Two wastes from the tyre recycling industry – the fibers used as reinforcing material and tyre crumbs – were pyrolyzed in two ovens of different configuration. Blends with a low rank coal and a bituminous waste were also prepared to modify the composition of the oils obtained from the pyrolysis of the tyre wastes. Elemental analysis, calorific value, Fourier transform infrared spectroscopy (FTIR) and gas chromatography were used to determine the oil composition. A comparative study taking into account the configurations of the ovens and the raw materials was carried out. The oils produced in the rotary oven were found to be more aromatic and to have lower oxygen contents. Depending on the type of oven and the material used in the co-pyrolysis process it is possible to obtain a fuel-oil with a specific heating value and sulfur content. It is also possible to obtain oil with more than 20% limonene and 20% BTX (benzene, toluene, xylene). The amount of aliphatics can be increased by including a coal in the pyrolysis process and the amount of aromatics can be increased by co-pyrolysis with a bituminous waste.

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BIODIESEL SYNTHESIS WITH ALKALINE CATALYSTS: A NEW REFRACTOMETRIC MONITORING AND KINETIC STUDY

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ABSTRACT

In this work, an experimental system was designed to allow the online monitoring of a chemical reaction in continuous flow leading to biodiesel synthesis using a portable digital refractometer. The proposed method was applied to the monitoring of the methanolysis of soybean oil using KOCH₃ as the catalyst at temperatures from 30 to 60 °C, allowing data acquisition in a relatively simple, reliable and cheap fashion. It was also possible to identify, discriminate and monitor the mixing (emulsification) and the reaction steps, with the former being the rate determinant. The methanolysis reaction is better represented by a zero-order kinetic scheme than by a pseudo-first-order scheme; the activation energy was determined to be $(31.3 \pm 1.8) \text{ kJ mol}^{-1}$. This behavior suggests that methanolysis with alkaline catalysts, usually considered as a homogeneous process, should in fact be assumed to be heterogeneous. Therefore, the rate of mixing controls the reaction kinetics and is a key factor in decreasing the transesterification time.

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PETROGRAPHIC CHARACTERIZATION OF COALS AS A TOOL TO DETECT SPONTANEOUS COMBUSTION POTENTIAL

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ABSTRACT

Textural features of 25 worldwide coals were studied after slow oxidation processing (0.5 °C min⁻¹ from 20 to 250 °C in air) using oil immersion microscopy and image analysis techniques. The characterization of samples, before and after oxidation, showed important changes in vitrinite reflectance with high reactive coals, which also related to their intrinsic self-oxidation potential. The morphology of the coal particles was also altered after the oxidation, to produce at least six different morphotypes. Particles with 'homogeneous change of reflectance' and particles with 'oxidation rims' were predominant in the samples studied, which related to boundary reactive conditions (kinetic and diffusion control of the reaction respectively). These textural characteristics indicate how particles interacted with oxygen at low temperatures, which could be used to predict the most probable pathway during the early stages of oxidation which could then lead to a spontaneous combustion event. The magnitude of the reflectance change and the morphological characteristics of samples studied were also related to the reactivity properties, providing an additional source of information to identify coals prone to spontaneous combustion.

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INFLUENCE OF VEGETABLE OIL FATTY ACID COMPOSITION ON ULTRASOUND-ASSISTED SYNTHESIS OF BIODIESEL

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ABSTRACT

Ultrasound is considered as one of the most attractive energies to assist biodiesel transesterification. The objective is to reduce the reaction time while saving energy. In the present study, four oils showing a wide range of fatty acid composition have been transesterified using ultrasound as auxiliary energy. Samples included unsaturated fatty acids (rapeseed and soybean) oils and saturated fatty acids (coconut and palm) oils. Transesterification reactions were conducted in batch and an ultrasound probe working under a fixed frequency of 20 kHz was used to facilitate the overall process. According to the design of experiments, variable duty cycle and amplitude, besides different concentrations of basic catalyst (KOH) and methanol-to-oil molar ratio were studied. The optimal fatty acid methyl ester (FAME) values were 95.03% for rapeseed biodiesel, 94.66% for soybean biodiesel, 81.37% for coconut biodiesel and 93.08% for palm biodiesel. A response surface methodology (RSM) was applied to determine the reaction parameters with a significant impact on response variables. Results showed that the length of chain and in a lower extent unsaturation degree of fatty acids have a significant effect on ultrasound assisted transesterification. In this sense, oils with higher unsaturation degree and long hydrocarbon chains provide higher FAME yields and lower glyceride concentrations than those with saturated fatty acids and short hydrocarbon chains.

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GASIFICATION KINETICS OF CHAR FROM OLIVE TREE PRUNING IN FLUIDIZED BED

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ABSTRACT

The gasification rate of char from olive tree pruning was measured in a fluidized bed at temperatures between 760 and 900 °C. Experiments were carried out using gas mixtures containing H₂O, CO₂, H₂, CO and N₂ in various proportions. Two kinetic equations were obtained, one for the char gasification rate with H₂O, taking into account the inhibition effect of H₂, and another for gasification with CO₂, including the inhibition effect of CO. The kinetic expressions account for the effect of temperature, gas composition, and the extent of carbon conversion. The influence of the gas composition and temperature was expressed by the Langmuir–Hinshelwood model, whereas an nth order kinetic model was used to account for the variation of the reaction rate with the extent of conversion. The reaction rate with H₂O was observed to be 3–4 times faster than that with CO₂. Inhibition effects caused by CO and H₂ were significant. It was found that the gasification rate in a mixture containing CO₂ and H₂O simultaneously can be estimated from addition of the individual rates with CO₂ and H₂O.

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THE EFFECT OF PARTICLE SIZE ON THE STRENGTH PARAMETERS OF GERMAN BROWN COAL AND ITS CHARS

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ABSTRACT

An experimental study on the compressive strength and Young's modulus of German brown coal from Schleenhain mine was carried out in order to determine the non-empirical mechanical properties required for the development of close-to-reality models of the stress-induced fragmentation of coal particles. A series of uniaxial compression tests was conducted on irregularly shaped coal specimens with diameters in the range of 0.8–6.3 mm, which are typical for industrial-scale coal utilization processes. According to the test results, the compressive strength and Young's modulus of coal particles significantly increase as the specimen size decrease. The data obtained show reasonable agreement with results published in the literature. Additionally, the mechanical properties of chars produced by coal pyrolysis at temperatures in the range of 400–1000 °C were measured in order to quantify the influence of the thermal treatment on mechanical properties. The compressive strength and Young's modulus of the chars increase to a maximum at a thermal treatment temperature of about 800 °C and then decrease as the temperature further increases.

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PYRIDINE HYDRODENITROGENATION OVER INDUSTRIAL NiMo/ γ - Al_2O_3 CATALYST: APPLICATION OF GAS PHASE KINETIC MODELS TO LIQUID PHASE REACTIONS

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ABSTRACT

A systematic methodology for simulating gas–liquid–solid kinetics starting from a gas–solid kinetics model has been developed and applied to pyridine hydrodenitrogenation over an industrial NiMo/ γ - Al_2O_3 catalyst. Data have been acquired in two independent, dedicated experimental programmes: i.e. an extended set of gas phase experiments that were previously carried out in a Berty type reactor setup at 573–633 K, 1.5–4.0 MPa and space times between 0.36 and 1.8 kg_{cat} s/mmol and a more limited set of liquid phase experiments that were performed as part of the present work in a Robinson–Mahoney reactor setup at 543–613 K, 6.0–8.0 MPa and space times between 0.65 and 3.0 kg_{cat} s/mmol. At liquid phase conditions the pyridine conversion ranged from 47% to 70%, while at gas phase conditions the pyridine conversion ranged from 17% to 72%. The reaction temperature and H₂S inlet partial pressure were found to be most significantly affecting the selectivity to intermediates and products in both experimental programmes. 1-pentylpiperidine formation, a bimolecular reaction product exclusively observed at liquid phase conditions, could be ascribed to the differences in phases present during the kinetic measurements as well as to the differences in molar H₂ and H₂S to pyridine inlet ratios used and the resulting surface concentrations. A kinetic model constructed using the gas phase data was extended to liquid phase conditions by accounting for (i) liquid phase non-ideality, (ii) solvent adsorption effects and (iii) the additionally observed response, i.e. 1-pentylpiperidine. The latter was found to be produced via condensation between piperidine and pentylamine.

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ESTIMATING THE ACTIVATION ENERGY OF EXOTHERMIC REACTIONS IN SUBSTANCES THAT UNDERGO SELF HEATING PROCESSES WITH THE HEAT RELEASE METHOD: USE OF SUB CRITICAL DATA

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ABSTRACT

Substance liable to self-heat and spontaneously ignite under storage or transportation conditions can be a serious fire hazard in several industries. In order to estimate if, under specific storage conditions, a substance will dangerously self heat up to ignition, it is necessary to have knowledge of several thermochemical properties of the substance itself. Among this properties, one of the most relevant is the overall activation energy of the exothermic reactions that are responsible of the internal heat generation. In this short communication it will be discussed the possibility to retrieve the value of the overall activation energy from oven heating experiments conducted at temperature below the critical temperature of the sample, taking as an example a set of experimental data retrieved for commercially available charcoal briquettes.

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REVIEW OF OIL SHALE SEMICOKE AND ITS COMBUSTION UTILIZATION

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ABSTRACT

This is the age of oil when many parts of the economy, particularly transportation, still rely heavily upon oil. The uncertainty in petroleum prices, its growing worldwide consumption and limited availability have motivated many countries rich in oil shale resources to investigate more efficient technologies to produce and use shale oil as an alternative to traditional petroleum. This review considers some aspects of oil shale based technologies. Among many differences in the flow and operational characteristics of several typical industrial oil shale retorting processes, one of the most important concerns how to treat semicoke and transfer the pyrolytic heat required for retorting oil shale. This will not only affect the yield and quality of shale oil, but also involves a series of serious issues related to energy and environment.

Semicoke, one of the final products formed after retorting oil shale, is a potentially harmful solid waste often containing some toxic organic compounds and heavy metals, disposal of which can result in very great environmental contamination. However, the organic compounds remaining in semicoke lead to it having a potential heat of combustion, and thus semicoke may be considered for combustion utilization as a fuel. This paper reviews the fundamental characteristics and combustion utilization possibilities for semicoke that would allow treating and utilizing semicoke efficiently and in an environmentally friendly manner. Although properties of semicoke vary widely with both the retorting processes and their operational parameters, it generally contains significant amounts of inorganic minerals from the oil shale matrix, some organic compounds and lesser amounts of trace elements. Its leaching elutes have shown acceptable limit values at a landfill for non-hazardous waste and thus the leaching of heavy metals is not necessarily a problem. However the leaching of organic compounds may often exceed the limits for dissolved organic carbon. Thus, the incineration of semicoke will often be desirable both to ensure relatively low harm to the environment as well as efficient resource recycling for energy. Based on the current status and probable future development of oil shale industries, and the combustion characteristics of semicoke, two technical routes have been recommended for utilizing semicoke. These might also be regarded as references or benchmarks for evaluating the new development of oil shale retorting processes. One method involves an integrated utilization system for oil shale in which semicoke is actively treated and utilized in a circulating fluidized bed boiler for providing heat for both retorting the oil shale and for generating steam. The other option is to employ circulating fluidized bed technology to burn semicoke which has been

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previously produced and might still be a byproduct of some retorting technologies. With regard to both options, industrial circulating fluidized bed combustion results are discussed, in an effort to establish the feasibility of burning semicoke in a circulating fluidized bed boiler.

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SYNERGISTIC EFFECT BETWEEN CO₂ AND H₂O ON REACTIVITY DURING COAL CHAR GASIFICATION

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ABSTRACT

In this study, the gasification reactivity of coal chars using CO₂/H₂O mixtures was investigated and the synergistic effect in reactivity between H₂O and CO₂ gasification was revealed. First, the coal samples were pyrolyzed under an argon atmosphere at four different temperatures (800–1100 °C in 100 °C increments). These four different char samples were then gasified isothermally at the four temperatures and five environments ranging from pure CO₂ to pure H₂O in 20 vol% increments. The results suggest that the addition of CO₂ improved the char reactivity, which is higher than the sum of the individual reactivity using either CO₂ or H₂O below 900 °C. At higher temperatures, H₂O gasification occurs most rapidly; however, its rate decreased with increasing volume fraction of CO₂. The high catalytic activity of Ca species in CO₂ gasification was the critical factor for the synergy between CO₂ and H₂O.

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SOOTING TENDENCY OF PARAFFIN COMPONENTS OF DIESEL AND GASOLINE IN DIFFUSION FLAMES

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ABSTRACT

The influence of the chemical structure on the sooting characteristics of some paraffin class hydrocarbons which are found in gasoline and diesel fuel is studied experimentally. The experiment involves the combustion of the paraffin in a wick-fed burner. Differential mobility spectrometry is used to measure the particle size distribution (PSD) at different flame heights. The wick-fed laminar diffusion flame is sampled at the tip; the flame height is modified systematically from small heights to large heights. Normal, iso and cyclo paraffins PSDs evolve in a similar way with flame height. At very low flame heights the PSD is unimodal, but rapidly evolves into a multi-modal one. The total number of particles peaks at small heights, and then decreases as flame height increase until it approaches constant values for all considered fuels. The mean soot particle diameter increases with flame height until a height where a maximum is achieved and sustained. Among each type of fuel, a systematic decrease in the maximum mean soot particle diameter was observed as the number of carbon atoms in the molecule increased. At all flame heights, comparing fuels with the same carbon number, cyclic paraffins presented the largest mean soot particles sizes, followed by iso-paraffins and the smallest particles for normal paraffins

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OXIDATIVE REMOVAL OF DIBENZOTHIOPHENE IN A BIPHASIC SYSTEM USING SOL-GEL FE/TIO₂ CATALYSTS AND H₂O₂ PROMOTED WITH ACETIC ACID

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ABSTRACT

Fe/TiO₂ catalysts were synthesized with the sol-gel method and were characterized by X-ray diffraction, N₂ adsorption measurement, Mössbauer spectroscopy, UV-vis spectroscopy, Raman spectroscopy, temperature programmed reduction, and temperature programmed desorption of NH₃. The Fe/TiO₂ catalysts chiefly consist of crystalline anatase. Fe³⁺ ions are highly dispersed on the surface and distributed in octahedral-coordinate sites within different environments in TiO₂. The Fe/TiO₂ catalysts were then evaluated for oxidation desulfurization of dibenzothiophene in a biphasic reaction mixture consisting of an acidified polar phase and a hexadecane model fuel phase. Compared to control tests, the catalytic activity for dibenzothiophene (DBT) oxidation is markedly improved by addition of acetic acid, typically at least doubling DBT conversion compared to that observed under control conditions. Under optimal conditions (10 wt% Fe in the Fe/TiO₂ catalyst and a pH adjusted to 0), 100% of the 300 ppm DBT initially present in the reaction mixture could be completely oxidized within 5 min. Oxidation of DBT formed sulfoxide/sulfones which were found to be enriched in the polar phase. The sol-gel Fe/TiO₂ catalysts possess several attributes which may contribute to their activity for DBT oxidation: (1) their hydrophilic-hydrophobic character that facilitates DBT oxidation as a phase transfer catalyst; (2) coordination and activation of acetic acid and peroxyacetic acid with Fe³⁺ and Ti⁴⁺ present at the Fe/TiO₂ surface, and (3) formation of superoxides at the Fe/TiO₂ surface.

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EVALUATION OF CORROSION CHARACTERISTICS OF ALUMINUM ALLOYS IN THE BIO-ETHANOL GASOLINE BLENDED FUEL BY 2-ELECTRODE ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY

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ABSTRACT

The corrosion characteristics of aluminum alloys were investigated in the bio-ethanol gasoline blended fuel at 100 ° C. The corrosion property of aluminum alloys was evaluated by an in situ 2-electrode electrochemical impedance spectroscopy (EIS), weight loss test and pressure-time measurement. Surface analysis was carried out after immersion test. The polarization resistance of aluminum alloys was increased at initial immersion time due to the formation of boehemite film (γ -AlOOH); after that, it was decreased due to the initiation of aluminum alkoxide reaction. The pressure of autoclave was increased because of the hydrogen gas from the aluminum-ethanol alkoxide reaction. It was verified that a 2-electrode EIS and pressure-time measurements were able to evaluate the corrosion resistance of aluminum alloys in the bio-ethanol gasoline blended solution.

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MAPPING INTERNAL STRUCTURE OF COAL BY CONFOCAL MICRO-RAMAN SPECTROSCOPY AND SCANNING MICROWAVE MICROSCOPY

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ABSTRACT

Structural complexity and variability of the chemical properties define technological applicability of coal and demand increasing accuracy and spatial resolution from the techniques used for coal characterization for development of new, clean, and efficient technologies of coal utilization. Here, we combined spatially-resolved reflectometry, fluorescence, and confocal micro-Raman spectroscopy with high-resolution scanning probe microwave imaging to achieve a nondestructive sub-100-nm spatial resolution mapping of coal structure. It was found that this approach allows for high spatial resolution identification of individual elements in coal architecture, thus potentially generating valuable input for knowledge-driven optimization and design of coal utilization processes.

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DETERMINATION OF EFFECTS OF VARIOUS ALCOHOL ADDITIONS INTO PEANUT METHYL ESTER ON PERFORMANCE AND EMISSION CHARACTERISTICS OF A COMPRESSION IGNITION ENGINE

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ABSTRACT

In this experimental study, effects of various alcohol additions into peanut methyl ester (PME) with ratio of 20% (by vol.) are investigated. After determining fuel properties of ethanol-methyl ester (EME), methanol-methyl ester (MME) and butanol-methyl ester (BME), their effects on engine performance and emissions are compared with PME and neat diesel fuel. It is observed that oxygen content of alcohols enhances combustion and increased engine power and torque values are achieved compared to PME. Also, improved combustion results in reduced carbon monoxide (CO) emissions and increased nitrogen oxides (NO_x). It is concluded that, average increments of 2.4%, 10% and 12.8% are obtained for MME, EME and BME, respectively compared to PME, in terms of engine power. Average increments of 1.2%, 3.4% and 6.1% are obtained for MME, EME and BME, respectively compared to PME, in terms of engine torque. Average reductions of 4.8%, 1.8% and 9.1% are achieved for MME, EME and BME, respectively compared to PME, in terms of CO emissions and average increments of 13.8%, 4.1% and 17.4% are achieved for MME, EME and BME, respectively compared to PME, in terms of NO_x emissions. On the other hand, average reductions of 26.36%, 20.85% and 18.91% are attained for MME, EME and BME, respectively compared to neat diesel fuel, in terms of engine power. Average reductions of 20.53%, 18.81% and 16.67% are acquired for MME, EME and BME, respectively compared to neat diesel fuel, in terms of engine torque. Average reductions of 12.17%, 9.37% and 16.14% are obtained for MME, EME and BME, respectively compared to neat diesel fuel, in terms of CO emissions and average increments of 18.49%, 8.26% and 22.19% are achieved for MME, EME and BME, respectively compared to neat diesel fuel, in terms of NO_x emissions.

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DISCRETE MULTICOMPONENT MODEL FOR BIODIESEL SPRAY COMBUSTION SIMULATION

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ABSTRACT

An important first step in spray combustion simulation is an accurate determination of the fuel properties which affects the modelling of spray formation and reaction. In a practical combustion simulation, the implementation of a multicomponent model is important in capturing the relative volatility of different fuel components. A Discrete Multicomponent (DM) model is deemed to be an appropriate candidate to model a composite fuel like biodiesel which consists of four components of fatty acid methyl esters (FAME). In this paper, the DM model is compared with the traditional Continuous Thermodynamics (CTM) model for both diesel and biodiesel. The CTM model is formulated based on mixing rules that incorporate the physical and thermophysical properties of pure components into a single continuous surrogate for the composite fuel. The models are implemented within the open-source CFD code OpenFOAM, and a semi-quantitative comparison is made between the predicted spray-combustion characteristics and optical measurements of a swirl-stabilised flame of diesel and biodiesel. The DM model performs better than the CTM model in predicting a higher magnitude of heat release rate in the top flame brush region of the biodiesel flame compared to that of the diesel flame. Using both the DM and CTM models, the simulation successfully reproduces the droplet size, volume flux, and droplet density profiles of diesel and biodiesel. The DM model predicts a longer spray penetration length for biodiesel compared to that of diesel, as seen in the experimental data. Also, the DM model reproduces a segregated biodiesel fuel vapour field and spray in which the most abundant FAME component has the longest vapour penetration. In the biodiesel flame, the relative abundance of each fuel component is found to dominate over the relative volatility in terms of the vapour species distribution and vice versa in the liquid species distribution.

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THE RESOURCE UTILIZATION OF OILY SLUDGE BY CO-GASIFICATION WITH COAL

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ABSTRACT

The utilization of oily sludge produced from refinery processes was evaluated in this study. Oily sludge was added to coal-water slurry (CWS) in different ways to prepare desirable coal-oily-sludge slurry (COSS). The slurryability and rheological characteristics of COSS were investigated and compared to CWS. The viscosity and yield stress of COSS sharply decrease with increasing the addition of oily sludge that preferentially wets coal particles. Microscopic structure and surface functional groups examination proved that oil droplets present in oily sludge could form a thin hydrophobic membrane on coal particle surface and modify its surface properties. The maximum solids loading can be either increased or decreased depending on the slurry preparation method. The maximum solids loading of COSS increases from 62.2 wt% to 64.0 wt% when oily sludge that preferentially wets coal was added in a ratio of 10.0 wt%.

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RELEASE OF ALKALI METAL, SULPHUR AND CHLORINE SPECIES DURING HIGH-TEMPERATURE GASIFICATION AND CO-GASIFICATION OF HARD COAL, REFINERY RESIDUE, AND PETROLEUM COKE

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ABSTRACT

Basic investigations using three different fuels as well as fuel blends have been performed in an atmospheric tube furnace at 1500 ° C under gasification like conditions. Molecular Beam Mass Spectrometry has been used for on-line analysis of the hot product gas. Main vapour species were H₂S, HCl, KOH, NaCl, COS, and KCl. After quantification of the data the release behaviour was correlated to the fuel composition. The released amount of HCl, NaCl, H₂S and COS of the blends hard coal/petroleum coke can be predicted by calculation. This can be explained by simple dilution effect. The released amount of HCl and NaCl of the blends hard coal/refinery residue can be predicted by calculation, but the released amount of H₂S and COS cannot be predicted.

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ABSORBANCE SPECTROMETRIC STUDY OF ELECTRON DONOR ACCEPTOR COMPLEXES OF COAL DERIVED ASPHALTENE WITH [60]- AND [70]FULLERENES

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ABSTRACT

Coal derived asphaltene (CDA) has been observed to form molecular complexes with electron acceptors such as [60]- and [70]fullerenes in carbon tetrachloride medium. The UV-vis spectroscopic studies show that CDA forms an inclusion complex of 2(CDA):1(fullerene) stoichiometry with [60]fullerene. On the other hand, CDA forms similar complex of 3(CDA):1(fullerene) stoichiometry with [70]fullerene. This is established by determining the thermodynamic parameters such as formation constants, enthalpies and entropies of the complex formation. The results also indicate that the process of complex formation in both the cases is entropy driven one.

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CONTINUOUS LIGNOCELLULOSIC ETHANOL PRODUCTION USING COLEUS FORSKOHLII ROOT HYDROLYSATE

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ABSTRACT

Root biomass of *Coleus forskohlii* obtained after extraction of forskolin constitutes more than 90% of the raw material rich in carbohydrates that could be used as a substrate for the production of bioethanol. Ethanol production from this waste biomass was optimized in batch and continuous fermentation. The maximum ethanol concentration of 31.32 g/l was obtained with batch fermentation. Continuous production of ethanol was carried out using wood chips immobilized cells of *Saccharomyces cerevisiae* in packed bed reactor. The maximum ethanol concentration of 34.25 g/l was obtained with nitrogen supplement and aeration as compared to 33.57 g/l without supplement and aeration at 0.1 (1/h) dilution rate showing no effect of aeration and nitrogen at low dilution rate. The maximum ethanol productivity (15.88 g/l h) was obtained at a dilution rate of 1 (1/h) with nitrogen supplement and aeration whereas ethanol productivity (13.48 g/l h) was obtained at a dilution rate of 0.75 (1/h) without nitrogen supplement and aeration showing promising effect of nitrogen and aeration at high dilution rate. Immobilized column reactor was useful for the production of bioethanol, and also suggests efficient utilization of *C. forskohlii* root biomass for the production of bioethanol.

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MONITORING THE DEGRADATION AND THE CORROSION OF NAPHTHENIC ACIDS BY ELECTROSPRAY IONIZATION FOURIER TRANSFORM ION CYCLOTRON RESONANCE MASS SPECTROMETRY AND ATOMIC FORCE MICROSCOPY

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ABSTRACT

Although the term “naphthenic acids” was originally used to describe acids that contain naphthenic rings, today this term is used in a more general sense and refers to all components in the acid extractable fraction. In crude oil, naphthenic acids exist as a complex mixture of compounds with broad polydispersity with respect to both molecular weight and structure. There has been increasing interest in the naphthenic acids in crude oil because of the corrosion problems that cause during oil refining. Herein, two powerful analytical tools, negative-ion electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry, ESI(-)FT-ICR MS and atomic force microscopy (AFM), were combined to monitor the thermal degradation of naphthenic acids and their corrosion effects on AISI 1020 steel, respectively. Two different acidic crude oils (TAN = 2.38 and 4.79 mg KOH g⁻¹, and total sulfur = 0.7993 and 1.0220 wt%) have been submitted to thermal treatment at 280, 300 and 350 ° C during 2, 4 and 6 h, and characterized by ESI(-)FT-ICR MS, total acid number (TAN), and total sulfur. The AISI 1020 steel was analyzed by scanning electron microscopy (SEM) and AFM. Generally, heating the crude oil at 350 ° C in a period of 6 h, it was observed that a high efficiency (≅80%) and selectivity of thermal decarboxylation process was monitored by decay of TAN (4.79 → 0.44 mg KOH g⁻¹). ESI(-)FT-ICR MS results showed that naphthenic acid species remained after the heating have DBE ranging 1-12 and carbon number from C₁₅ to C₄₅. AFM topographic profile evidenced that the naphthenic acid corrosion of the crude oil with TAN of 4.73 mg KOH g⁻¹ on AISI 1020 steel was profoundly altered and a marked reduction in peak to peak height values (obtained by subtracting the value of the lowest peak by the highest peak in the topographic area examined). Optical images and microphotographs confirmed the presence of irregularities, characterizing the corrosion mechanism as pitting type. The naphthenic corrosion was also evidenced in samples with low TAN value (0.44 mg KOH g⁻¹).

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D-LOADED MESOPOROUS SILICA AS A ROBUST ADSORBENT IN ADSORPTION/DESORPTION DESULFURIZATION CYCLES

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ABSTRACT

Desulfurization of benzothiophene/isooctane mixtures and gasoline (42.5 and 1000 ppmw S) was studied by batch and fixed bed experiments using PdCl₂ supported on mesoporous silica of SBA-15 type (PdCl₂/SBA-15). The Pd-loaded silica was prepared by solid-phase impregnation of the metal halide on the mesoporous siliceous matrix (SBA-15). SBA-15 and PdCl₂/SBA-15 were characterized with N₂ adsorption/desorption isotherms, small angle X-ray diffraction and transmission electron microscopy (TEM). Then desulfurization of benzothiophene/isooctane mixtures and gasoline (42.5 ppmw S) with these sorbents was investigated by batch and fixed bed experiments. PdCl₂/SBA-15 showed much higher capacity for sulfur adsorption than both the starting material and PdCl₂ itself. A mathematical model was used to represent the breakthrough curves for adsorption and desorption runs in fixed bed, providing very good agreement between numerical simulations and adsorption data. The spent PdCl₂/SBA-15 was regenerated using isooctane as eluent, and the regenerated PdCl₂/SBA-15 was tested again for the desulfurization of 1000 ppm S gasoline (down to 50 ppm). The results showed that the sulfur adsorption capacity at the break point ($C = 50$ ppm) remained nearly unchanged for three cycles, even though XPS elemental analysis for the fresh and spent adsorbent revealed some degree of leaching of the metal from the external surface, particularly as Pd(II). In conclusion, PdCl₂/SBA-15 appears to be a robust adsorbent for desulfurization of liquid fuels and the model proposed herein was able to predict deep desulfurization of gasoline in cyclic mode.

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EFFECT OF PARTICLE HYDROPHOBICITY ON CO₂ FOAM GENERATION AND FOAM FLOW BEHAVIOR IN POROUS MEDIA

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ABSTRACT

Studies of CO₂ foam stabilized with silica nanoparticles at reservoir conditions were carried out for CO₂ foam enhanced oil recovery (EOR) application. In the study described in this paper, three types of silica nanoparticles with varied wettability were employed to study the effects of particle hydrophobicity on CO₂ foam generation at reservoir conditions. The results showed that nanoparticle surface hydrophobicity played an important role in CO₂ foam generation. More CO₂ foam was generated as the particle surface changed from strongly hydrophilic to somewhat hydrophobic. The bubble size of the CO₂ foam decreased noticeably as the particle surface became more hydrophobic. Nanosilica particle-stabilized CO₂ foam demonstrated a significant effect on the reduction of the CO₂ mobility at a phase ratio between 2 and 11. The particle-stabilized CO₂ foam also improved the apparent viscosity of s

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PRODUCTION AND CHARACTERIZATION OF PYROLYTIC OIL BY CATALYTIC PYROLYSIS OF NIGER SEED

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ABSTRACT

Conventional pyrolysis of Niger seed was investigated in a semi batch reactor with and without the presence of catalyst. Thermal pyrolysis yielded maximum 34.5% of oil (by weight basis) at 550 ° C temperature. The catalytic pyrolysis was carried out using catalysts Al₂O₃, CaO and Kaolin at 2:1, 4:1 and 8:1 feed to catalyst ratio at this temperature. The yield and fuel properties of thermal and catalytic pyrolytic oils were compared. The results confirmed that the presence of catalysts decreased the oil yield marginally whereas enhanced the fuel properties compared with thermal pyrolysis. It was observed that the three catalysts had different effect on the fuel properties of pyrolytic oils. Among the three different feed to catalyst ratios used, 8:1 resulted in higher oil yield and thus the fuel properties were evaluated at this ratio. Kaolin at 8:1 ratio was more suitable to enhance calorific value whereas CaO at 8:1 ratio was able to reduce the viscosity of pyrolytic oil. The FTIR and DSC analysis confirmed that pyrolytic oil was a mixture of saturated and unsaturated hydrocarbon compounds.

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CHEMICAL COMPOSITIONAL AND STRUCTURAL CHARACTERISTICS OF LATE PERMIAN BARK COALS FROM SOUTHERN CHINA

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ABSTRACT

The characteristics of an unusual liptinitic component, known in Chinese petrographic nomenclature as barkinite, have been studied over the past 80 years. The chemical characteristics of barkinite have been studied for many years, but there has been little progress in establishing the chemical structural differences between barkinite and other liptinitic macerals of the same rank and age. In this paper, aspects of the chemical composition and structural characteristics of bark coal/barkinite are discussed. Bark coal is high volatile bituminous coal and has high volatile matter yield (>37%, daf, dry-ash free). The hydrogen content and H/C atomic ratio of barkinite are higher than those of vitrinite. The classification of barkinite would be type I-II kerogen. In addition, the chemical structure of barkinite is characterized by rich aliphatic structure concentration although dominated by aromatic structure. Chemical structural characteristics of barkinite seem close to vitrinite.

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INFLUENCE OF ETHANOL ADDITION IN REFINERY STREAM FUELS AND THE HCCI COMBUSTION

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ABSTRACT

The auto-ignition, stability and duration of the combustion process in an HCCI engine, depend on the interplay between the in-cylinder thermal environment and a given fuel's chemical kinetics. Fuel available in the US market differs appreciably in composition and auto-ignition chemistry, hence strategies intended to bring HCCI to mass production must account for this fuel variability.

To address this issue, a test matrix of eight gasoline fuels, comprised of blends made from refinery streams, was created, and these eight fuels were run in an experimental, single cylinder HCCI engine. The properties of these fuels vary according to their volumetric concentration of ethanol, sensitivity ($S = \text{RON} - \text{MON}$) and volumetric content of aromatics and olefins. The fuels all have similar RON ratings, and were designed, in large part, to mimic commercial pump gasoline available in the United States. The ethanol content was increased to 20% by volume in some fuels, specifically to investigate the impact of the oxygenate fraction on HCCI. This concentration is higher than what is currently available on average at the pump, but is relevant in the context of recent discussions about raising the ethanol content of gasoline, in the near future.

For each fuel, several types of experiments were conducted to assess the effects of increased ethanol content on HCCI combustion. Since it is not practical to investigate the ignition delay, the first set of experiments was a compensated load sweep, in which combustion phasing was matched across a sweep of fuelling rate by adjusting the intake air temperature. Next, the limits of HCCI operability across the speed range were established, by varying load until either the misfire or ringing limit was detected. Finally, air temperature sweeps were carried out to correlate fuels' properties and the sensitivity of HCCI with the in-cylinder thermal environment. Increased ethanol content led to a number of important changes in engine performance, including, but not limited to, specific fuel consumption, HCCI operating range and variation of combustion phasing over a range of intake charge temperature.

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NITROGEN DOPING OF ASH-FREE COAL AND EFFECT OF ASH COMPONENTS ON PROPERTIES AND OXYGEN REDUCTION REACTION IN FUEL CELL

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ABSTRACT

Nitrogen doping of ash-free coal (HPC) and raw coal in a stream of ammonia was studied in application to a cathode catalyst for a fuel cell. The relation to structure morphology, surface properties and catalytic activity for the oxygen reduction reaction (ORR), the effects of addition of the ash components of the raw coal to HPC and the comparison with carbonization in a stream of helium were determined. Tests were carried out with linear sweep voltammetry measurement in streams of oxygen and argon gases and a scan region of 0.04–1.04 V using a three-electrode setup. Inorganic elements dominant in the ash of the raw HPC coal were iron, aluminum, potassium, magnesium, silicon and calcium. The nitrogen doping of HPC at 773–1073 K decreased the oxygen content and increased the nitrogen content and the pyridinic nitrogen with the treating temperature compared to the carbonization in a stream of helium based on the XPS analysis. The addition of metals to HPC and subsequent nitrogen doping decreased the nitrogen content of HPC but increased the pyridinic nitrogen in the nitrogen distribution except for magnesium and calcium due to interaction with the pyridinic nitrogen. From the Raman analysis, the nitrogen doping at 773–1073 K decreased the I_D/I_G ratio (deficient carbon degree) compared to the carbonization, but the addition of the ash components, especially 0.5% Fe + 0.5% Al, increased it, resulting from the formation of many edges of deficient carbons in the presence of the ash. The TEM observation showed that the nitrogen doping of HPC at 1073 K created onion-like fullerene structures but the addition of iron and aluminum destroyed this structure and formed a nanocarbon structure. The presence of iron and aluminum increased the pyridinic nitrogen and the disordered defect carbons formed along the edges of the graphite layers. Furthermore, the nitrogen doping at 1073 K increased the onset potential of the ORR from 0.37 (carbonizing) to 0.67 V. The addition of both iron and aluminum further increased the onset to 0.79 V for the ORR which was the same potential as that of the raw HPC containing the ash components. The presence of ash in the raw coal, especially iron and alumina, promoted the electronic performance for the oxygen reduction. Consequently, the nitrogen-doped combined iron and aluminum with nanocarbons were the active species of the HPC catalysts for the ORR.

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ESTIMATION OF SURFACE TENSION OF FATTY ACID METHYL ESTER AND BIODIESEL AT DIFFERENT TEMPERATURES

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ABSTRACT

Surface tension (γ) is an important physical property of biodiesel for atomization and complete combustion in the diesel engine. In this study, the Martin's rule of free energy additivity is extended to cover the free energy of interfacial interaction of a liquid. Finally, an equation ($\gamma = 60.211 - 0.4307z - 0.1125T + 0.00207zT + 3.676m - 0.00893mT$) is derived for estimation of the surface tension of an individual fatty acid methyl ester (FAME), where T , z and m are absolute temperature, number of carbon atoms and number of double bond(s) of fatty acid, respectively. When the proposed equation was used for estimation of the surface tension of FAMEs, the deviation range was 0.03–5.54% and the average absolute deviation (AAD) was 1.32% at temperature between 20 and 100 °C.

Also, the proposed equation can be used for estimation of the surface tension of a biodiesel. In this case, the average carbon numbers (z_{avg}) and average number of double bonds (m_{avg}) must be used in place of z and m , respectively. Thus, the prior knowledge of surface tension of individual FAME is not necessary. The estimated surface tensions of biodiesels at temperatures between 30 and 80 °C were in good agreement with the literature values. The deviation range was 0.10–5.70% and the AAD was 2.09%.

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AUTOIGNITION OF KEROSENE (JET-A)/AIR MIXTURES BEHIND REFLECTED SHOCK WAVES

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ABSTRACT

Ignition delay times have been measured for gas-phase mixtures of aviation kerosene Jet-A with air at pressures of 10 and 20 atm. The experiments have been carried out in a heated shock tube at a heating temperature of 150 °C. The measurements have been performed for the lean, stoichiometric and rich mixtures (ϕ 0.5; 1; 2) behind the reflected shock wave in the temperature range of 1040–1380 K. Ignition delay times have been measured using OH emission at 309 nm and —CH₃ absorption at 3.39 μ m. The obtained results are in agreement with the results of other groups. The experimental data have been summarized in a single expression:

$\tau_{\text{ign}} = 1.31 \times 10^{-3} [\mu\text{s}] \cdot (P/1[\text{atm}])^{-0.67} \cdot \phi^{-0.6} \cdot \exp(30.4[\text{kcal/mol}]/RT)$,
where ϕ is the equivalence ratio. The measured ignition delay times for Jet-A/air mixtures are given in Annex tables.

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DEVELOPMENT OF A GAS PHASE COMBUSTION MODEL SUITABLE FOR LOW AND HIGH TURBULENCE CONDITIONS

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ABSTRACT

A novel hybrid gas phase combustion model suitable for low as well as high turbulent combustion conditions is proposed. In particular, in the region above the fuel bed of small-scale biomass combustion plants, gas phase mixing is highly influenced by laminar and low turbulence zones. Here, the eddy break-up combustion models are not valid because they were originally developed for highly turbulent flows. Therefore, a CFD gas phase reaction model applicable over the whole Reynolds range from laminar to turbulent flows is developed. It is a hybrid Eddy Dissipation Concept/finite rate kinetics model which calculates the effective reaction rate from laminar finite rate kinetics and the turbulent reaction rate and weights them depending on the local turbulent Reynolds number of the flow. To validate the proposed model, comparisons are made with experimental data for a series of jet flames covering laminar, transitional, and turbulent flow conditions. The simulation results show that the prediction of flame can be improved with the proposed hybrid combustion model.

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SPECIATION OF ORGANIC SULFUR COMPOUNDS USING COMPREHENSIVE TWO-DIMENSIONAL GAS CHROMATOGRAPHY COUPLED TO TIME-OF-FLIGHT MASS SPECTROMETRY: A POWERFUL TOOL FOR PETROLEUM REFINING

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ABSTRACT

Sulfur compounds are among the most important heteroatomic constituents of petroleum. These compounds are undesirable because they increase emulsion stability, cause corrosion, contaminate catalytic processes of refining, and determine color and odor of final products. Also, sulfur compounds play an important role in naphthenic corrosion, which occurs via chemical reaction of naphthenic acids with iron; sulfur limits corrosion through formation of a surface film of FeS, but this formation does not occur for all classes of sulfur compounds. Hence, their speciation is important. In this work, qualitative and semi-quantitative characterization of organic sulfur compounds were performed in two petroleum samples with no pre-treatment using comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry (GC × GC-TOFMS). Total sulfur content (ASTM D 4294) was 1.91% and 0.96%, on mass %, while ° API was 33.1 and 19.6 for sample #1 and sample #2, respectively. Regarding cyclic sulfur compounds, one sample showed a total concentration of 60,363 $\mu\text{g g}^{-1}$ of whole oil, while the other sample showed a total concentration of 4,740 $\mu\text{g g}^{-1}$. Further, sulfides, disulfides, and thiols were detected only in sample #1; total concentration was 1,372 $\mu\text{g g}^{-1}$. Thus, total concentration of all sulfur compounds for sample #1 was 61,735 $\mu\text{g g}^{-1}$. These data illustrate the potential of the GC × GC-TOFMS technique for molecular characterization and semi-quantification, in this case sulfur speciation, of complex samples, such as petroleum.

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FUNDAMENTAL COMBUSTION CHARACTERISTICS OF JATROPHA OIL AS ALTERNATIVE FUEL FOR GAS TURBINES

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ABSTRACT

To investigate the combustion characteristics of Jatropha pure oil (JPO) and Jatropha methyl ester (JME) as an alternative fuels for gas turbines, combustion experiments were conducted at atmospheric pressure employing an air-assist pressure swirl atomizer. As well as the NO_x and CO concentrations and smoke number in the exhaust gas, the flame radiation intensity was measured using the two-color method. The results show that the flame radiation intensity and the soot emission decrease with increasing mixing ratio of JPO or JME to diesel fuel. It was also found that the flame radiation intensity has a strong correlation with the mean diameter of the fuel spray for all fuels. The CO emission for JPO is higher than those for JME and diesel fuel in the case of low flame temperature.

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THE GENETIC ALGORITHM BASED BACK PROPAGATION NEURAL NETWORK FOR MMP PREDICTION IN CO₂-EOR PROCESS

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ABSTRACT

In this study, a genetic algorithm based back propagation artificial neural network model was developed and used to predict the minimum miscibility pressure, i.e. MMP, for both pure and impure CO₂ injection cases. Ten parameters that affecting the MMP were chosen as input variables, while the MMP was selected as output parameter. These parameters were reservoir temperature-TR, mole fraction of volatile oil components-xvol, mole fraction of intermediate oil components-xint, mole fraction of C5-C6 oil components-xC5-C6, molecular weight of C7+components-MWC7+, mole fraction of CO₂ in solvent-xCO₂, mole fraction of C1 in solvent-xC1, mole fraction of N₂ in solvent-xN₂, mole fraction of H₂S in solvent-xH₂S, and mole fraction of C2-C4 in solvent-xC2-C4. The performance of the newly developed model was evaluated by calculating the deviations between the predicted and the target values, and was compared with four well known correlations in published literature. Through the comparison, it can be found that our new model outperformed those four correlations with the lowest average absolute relative error of 5.51% and mean square error of 7.01%. The influence degrees of each factor on MMP were also analyzed qualitatively and quantitatively by sensitivity analysis. It was found that xint, xC5-C6, and xH₂S have positive effects on MMP, while TR, xvol, MWC7+, xCO₂, xC1, and xN₂ have negative effects on MMP. In addition, the effect of xC2-C4 on MMP can be neglected. Furthermore, the variations of MMP with the increase of each factor were also considered, and it can be found that the slopes of these curves are not constant all the time and change with the variations of the influence factors.

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STABILITY OF ACETYLENE-PROPANE-BUTANE AND ACETYLENE-HYDROGEN GAS MIXTURES SUBJECTED TO SHOCK WAVE ACTION

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ABSTRACT

Inhibition of exothermal spontaneous decomposition of acetylene by dilution with a gaseous propane-butane mixture or with hydrogen, which themselves serve as fuels, was carried out experimentally. Mixtures of acetylene with the inhibitors, located in a cylindrical shock tube, were heated by a reflected shock wave. The source of the shock wave was provided by a detonation wave initiated in a stoichiometric acetylene-oxygen mixture and then converted to a shock wave in the acetylene-inhibitor mixture. Minimal limits of bulk concentrations of inhibitors were obtained over a range of initial pressure 0.1-0.25 MPa at which no spontaneous decomposition of acetylene occurred.

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SAWDUST AGE AFFECT ALDEHYDE EMISSIONS IN WOOD PELLETS

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ABSTRACT

The environmental and energy policies in most nations worldwide aim at replacing fossil fuels with renewable sources of energy. The use of wood pellets made from sawdust is rapidly increasing. Wood pellets are a refined compacted fuel with high energy density and low emissions during combustion. Sawdust and wood pellets may be stored for several months due to seasonal demand variation and wood-fuel trade. Wood contains unsaturated fatty acids susceptible to oxidation, a process commonly referred to as fats going rancid. The level of oxidation in pellets is an important parameter of pellets quality as oxidation during storage causes problems such as self-ignition of pellets stored in silos and emissions of malodorous compounds. The purpose of this work was to investigate the effect of the age of the raw material on the oxidation caused aldehyde emissions from wood pellets. Pellets were produced from Scots pine (*Pinus sylvestris*) sawdust that was either freshly sawn or had been stored for 4 months. The pellets were then stored in either 18 ° C or in 40 ° C. The formation of the aldehyde hexanal was analyzed with static headspace and gas chromatography. Pellets made from fresh sawdust were low-emitting after 80 days, whereas pellets made from aged sawdust did not reach the same low level until 190 days after production. This held true whether the pellets were stored in 18 ° C or in 40 ° C. The aged sawdust pellets had maximum emissions at the same time as the emissions ceased from the fresh sawdust pellets. A key conclusion is that when a low level of aldehyde emissions is required during storage, the pellets should be produced of sawdust that is freshly sawn.

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LINK BETWEEN ENDOWMENTS, ECONOMICS AND ENVIRONMENT IN CONVENTIONAL AND UNCONVENTIONAL GAS RESERVOIRS

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ABSTRACT

This paper presents a methodology for connecting endowments, economics and the environment in conventional, tight, shale and Coalbed Methane (CBM) reservoirs. The volumetric estimates are generated by a Variable Shape Distribution model (VSD). The VSD has been shown in the past to be useful for the evaluation of conventional and tight gas reservoirs. However, this is the first paper in which the method is used to also include shale gas and CBM formations. Results indicate a total gas endowment of 70,000 tcf, split between 15,000 tcf in conventional reservoirs, 15,000 tcf in tight gas, 30,000 tcf in shale gas and 10,000 tcf in CBM reservoirs. Thus, natural gas formations have potential to provide a significant contribution to global energy demand estimated at approximately 790 quads by 2035.

A common thread between unconventional formations is that nearly all of them must be hydraulically fractured to attain commercial production. A significant volume of data indicates that the probabilities of hydraulic fracturing (fracking) fluids and/or methane contaminating ground water through the hydraulically-created fractures are very low. Since fracking has also raised questions about the economic viability of producing unconventional gas in some parts of the world, supply curves are estimated in this paper for the global gas portfolio. The curves show that, in some cases, the costs of producing gas from unconventional reservoirs are comparable to those of conventional gas.

The conclusion is that there is enough natural gas to supply the energy market for nearly 400 years at current rates of consumption and 110 years with a growth rate in production of 2% per year. With appropriate regulation, this may be done safely, commercially, and in a manner that is more benign to the environment as compared with other fossil fuels.

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ON THE USE OF A HIGHLY REACTIVE IRON ORE IN CHEMICAL LOOPING COMBUSTION OF DIFFERENT COALS

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ABSTRACT

Coal combustion using the Chemical Looping technology can be carried out under different configurations. This paper focuses on the *in situ* gasification Chemical Looping Combustion (iG-CLC). In this technology, it is especially important the selection of the oxygen carrier as there may be losses in the drainage of coal ashes. Finding low-cost oxygen carriers has become a relevant research focus. Several Fe-based materials have been tested including minerals and industrial residues. In this work, a highly reactive iron ore that had already shown promising characteristics for coal combustion was used in a continuous 500 W_{th} CLC unit. Its performance in the combustion of anthracite, bituminous coal and lignite was evaluated and compared with the results for other Fe-based materials, such as ilmenite or a bauxite waste. The combustion efficiency obtained with the Tierga iron ore was the highest reported to date which makes this carrier a promising candidate for further scale-up. Moreover, the high CaO content of this material led to analyze its relevance for sulphur removal during the first hours of operation. High sulphur retention capacity was observed but this capacity decreased with time as the calcium oxide was both saturated and lost as fines during operation.

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THERMAL CRACKING OF FREE FATTY ACIDS IN INERT AND LIGHT HYDROCARBON GAS ATMOSPHERES

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ABSTRACT

The aim of this work was to study the pyrolytic conversion of free fatty acids to renewable hydrocarbons in the presence of short-chain alkane and alkene hydrocarbon gases. Oleic acid (cis-9-octadecanoic acid) was used as model for fatty acids produced from hydrolysis of lipids from animal and plant feedstock. Batch pyrolysis reactions were conducted at 410 ° C for 2 h at an initial pressure between 130 psi (896.3 kPa) and 500 psi (3447.4 kPa) under constant agitation. Identification and quantification of the pyrolysates in the gas and liquid phase were carried out using gas chromatography and mass spectrometry. Under inert N₂ atmosphere liquid product yields were between 74 and 81 wt% of feed with lower pressure giving the highest product yields. Liquid product was composed mainly of alkanes and alkenes ranging in carbon number from 6 to 19 and fatty acids from carbon numbers 4 to 18. Pyrolysis reactions conducted in the presence of short-chain alkane gases did not appreciably influence the liquid product yield and the composition compared to the inert atmosphere. On the other hand, pyrolysis reaction in presence of short-chain alkene gases resulted in a marked increase in the liquid product yield, the production of branched alkanes and alkenes and increased fatty acid decarboxylation. This work demonstrates a novel approach to concurrently increase the liquid product yield in pyrolysis of free fatty acids and produce highly valuable branched hydrocarbons for fuel and solvent applications.

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THE ROLE OF DIMETHYL ETHER AS SUBSTITUENT TO ETHYLENE ON PARTICULATE FORMATION IN PREMIXED AND COUNTER-FLOW DIFFUSION FLAMES

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ABSTRACT

The role of dimethyl ether (DME) as substituent to ethylene on particulate formation has been evaluated in premixed and counter-flow diffusion flames. In the premixed flame, the equivalence ratio has been changed from 1.95 to 2.61 and dimethyl ether has been added from 2% to 30% of the total carbon fed. In the counter-flow diffusion flame, the addition of DME has been from 0% to 60% of total carbon fed. Laser induced fluorescence and incandescence have been used to follow the soot formation process: UV and visible fluorescence signals have been attributed to aromatic macromolecules and incipient nanoparticles, respectively, whereas incandescence has been attributed to soot particles and aggregates.

In premixed flames results evidence that the formation of soot precursors is not so sensitive to DME addition. In very rich combustion environments, DME addition cannot completely avoid the formation of small precursors, although it can slow down the formation process. This behavior has been observed for all the equivalence ratios investigated.

In the pyrolysis region of counter-flow diffusion flames, the formation of aromatic small precursors and soot particles is increased for small DME percentages, up to 20%. Then, the precursors are suppressed for larger amounts, going below the detection limit when 60% of DME is used. This suggests that DME can enhance the production of radicals and small reactive molecules in the pyrolytic side when it is added in small concentrations. For larger amounts of DME, oxidative pathways prevail and the conversion of carbon to precursors and then to soot is inhibited. In the oxidative region DME starts to effectively decrease the particle reduction also for amounts as small as 10–15%.

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HYDROCRACKING OF EXTRA-HEAVY OIL USING CS-EXCHANGED PHOSPHOTUNGSTIC ACID ($\text{Cs}_x\text{H}_{3-x}\text{PW}_{12}\text{O}_{40}$, $x = 1-3$) CATALYSTS

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ABSTRACT

In this study, Cs-exchanged phosphotungstic acids ($\text{Cs}_x\text{H}_{3-x}\text{PW}_{12}\text{O}_{40}$, $x = 1-3$) were examined as a catalyst for the hydrocracking of extra-heavy oil (vacuum residue, API gravity = 2.3°). $\text{Cs}_x\text{H}_{3-x}\text{PW}_{12}\text{O}_{40}$ showed a higher activity than the commercially available, NiMo/ Al_2O_3 -based catalyst in the hydrocracking of extra-heavy oil; the former catalyst produced a larger quantity of liquid oils than the commercial catalyst. The liquid oils produced by the phosphotungstic acids were slightly heavier than those produced by the commercial catalyst. They also showed comparable activities to the commercial catalyst in terms of the hydrogenative removal of metals (nickel, vanadium) and sulfur from the extra-heavy oil. It was found that the hydrocracking performance was primarily dependent on the surface acid density of heteropolyacids. The best performance of the $\text{Cs}_x\text{H}_{3-x}\text{PW}_{12}\text{O}_{40}$ catalysts was obtained at a Cs loading of $x = 2.2$, where the surface acid density was highest. To assess the physical and chemical properties of the catalysts, various characterization techniques were used, including inductively coupled plasma-mass spectrometry, X-ray diffraction, thermogravimetric analysis, Fourier transform-infrared spectroscopy, Brunauer-Emmett-Teller analysis, and ammonia-temperature programmed desorption analysis.

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IGNITION DELAY TIMES OF VERY-LOW-VAPOR-PRESSURE BIODIESEL SURROGATES BEHIND REFLECTED SHOCK WAVES

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ABSTRACT

Ignition delay times for a variety of low-vapor-pressure biodiesel surrogates were measured behind reflected shock waves, using an aerosol shock tube. These fuels included methyl decanoate ($C_{11}H_{22}O_2$), methyl laurate ($C_{13}H_{26}O_2$), methyl myristate ($C_{15}H_{30}O_2$), methyl palmitate ($C_{17}H_{34}O_2$), and a methyl oleate ($C_{19}H_{36}O_2$)/Fatty Acid Methyl Ester (FAME) blend. Experiments were conducted in 4% oxygen/argon mixtures with the exception of methyl decanoate which was studied in 1% and 21% oxygen/argon blends. Reflected shock conditions covered initial temperatures from 1026 to 1388 K, pressures of 3.5 and 7.0 atm, and equivalence ratios from 0.3 to 1.4. Arrhenius expressions describing the experimental ignition delay time data are given and compared to those derived from applicable mechanisms available in the literature. Graphical comparisons between experimental data and mechanism predictions are also provided. Experiments of methyl laurate, methyl myristate, and methyl palmitate represent the first shock tube ignition delay time measurements for these fuels. Finally, experiments with methyl palmitate represent, to the authors' knowledge, the first neat fuel/oxidizer/diluent gas-phase shock tube experiments involving a fuel which is a waxy solid at room temperature.

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LOW TEMPERATURE OXIDATION OF N-HEXANE IN A FLOW REACTOR

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ABSTRACT

The risk of igniting a flammable mixture in fuel tank vapor space is a major concern in aviation safety. In order to analyze the hazards and develop mitigation strategies, it is necessary to characterize the explosive properties of kerosene vapor–air mixtures over wide ranges of initial conditions. n-Hexane has been extensively used in our laboratory as a single component surrogate of kerosene. In the present study, hexane oxidation by oxygen was studied in a flow reactor at equivalence ratios of 0.7, 1 and 1.5 for mixtures diluted at 90% with nitrogen. Residence time was set at 2 s and the pressure at 100 kPa. The evolution of the gas phase composition at the reactor exit was studied over the range 450–1000 K. Laser-based diagnostics and gas chromatography analysis were used to characterize the exit mixture composition. The chemical species measurements revealed three distinct regimes of oxidation, namely (i) the cool flame region from 600 to 650 K, (ii) the NTC region between 675 and 775 K, and (iii) the high temperature oxidation regime from 800 K. The modeling study demonstrated the capability of reproducing most of the trends observed experimentally.

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PLASMA ASSISTED POWER COAL COMBUSTION IN THE FURNACE OF UTILITY BOILER: NUMERICAL MODELING AND FULL-SCALE TEST Q

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ABSTRACT

This work presents modern plasma technology for solid fuel ignition and combustion. It promotes more effective and environmentally friendly low-rank coal incineration. To implement this technology at coal fired thermal power plants plasma-fuel systems (PFSs) were developed. PFS is a pulverized coal burner equipped with arc plasmatron producing high temperature air stream of 4000–6000 °C. Basis of technology PFS is plasma thermo-chemical preparation of coal for burning. It consists in plasma heating of air–coal mixture up to temperature of coal volatiles release and char carbon partial gasification. In PFS air–coal mixture is deficient in oxygen therefore carbon is oxidized mainly to carbon monoxide. As a result, at the PFS exit a highly reactive mixture is formed of combustible gases and partially burned char particles, together with products of combustion, while the temperature of the mixture is around 1050 °C. Further mixing with air promotes intensive ignition and combustion of the prepared in the PFS fuel.

PFS have been tested for boilers start up and pulverized coal flame stabilization at 30 power boilers of 75–950 t/h steam productivity. The boilers were equipped with different types of pulverized coal burners: direct flow, muffle and swirl burners. At tests of the PFS power coals of all ranks (lignite, bituminous, anthracite and their mixtures) were incinerated. Volatile content of them was in range of 4–50%, ash varied from 15% to 48% and heat of combustion was from 6690 to 25100 kJ/kg.

To show advantages of the plasma technology of coal combustion before conventional one numerical investigation of plasma ignition, gasification and thermo-chemical preparation of air–coal mixture for incineration in a power boiler was fulfilled. The numerical modeling was performed for low-rank bituminous coal of 40% ash content incinerated at a boiler of 420 t/h steam productivity. Both analysis of the numerical modeling and experience of PFS industrial use showed ecological efficiency of the plasma technology. When plasmatrons operate in the regime of plasma stabilization of pulverized coal flame, NO_x emission is reduced twice and amount of unburned carbon is reduced four times. The PFSs reduce the temperature at the exit of the furnace. Tests of the PFS for the boiler BKZ-420 of Almaty TPP-2 cold startup confirmed the possibility of high-ash Ekibastuz coal ignition in the cold furnace without heating of primary air.

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THE ENTRAINMENT BEHAVIOUR OF SERICITE IN MICROCRYSTALLINE GRAPHITE FLOTATION

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ABSTRACT

Few publications focus on the influence of hydrophobic minerals such as graphite or coal on entrainment behaviour of hydrophilic gangue, although they coexist with one another in flotation pulp. This paper presented an experimental study on entrainment behaviour of sericite in the absence and presence of hydrophobic microcrystalline graphite, and explained the poor flotation selectivity of microcrystalline graphite ore.

For sericite and microcrystalline graphite single mineral, batch flotation tests and contact angle measurements were conducted, the results indicated that hydrophilic sericite was easy to entrain into concentrate and this process was strongly affected by its particle size; the particle size and solid concentration of hydrophobic graphite intensely affected water recovery of concentrate. Batch flotation tests of artificial mixtures composed of sericite and microcrystalline graphite were also carried out. The results indicated that the particle size and concentration of hydrophobic graphite significantly affected the recovery of water, the entrainment factor of sericite, and the recovery of sericite in concentrate. The serious entrainment or entrapment of sericite in the presence of hydrophobic microcrystalline graphite leads to poor selectivity in microcrystalline graphite ore flotation.

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EXTRACTION OF ALUMINIUM FROM COAL FLY ASH: IDENTIFICATION AND OPTIMIZATION OF INFLUENTIAL FACTORS USING STATISTICAL DESIGN OF EXPERIMENTS

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ABSTRACT

In this study, a statistical Design of Experiments (DOE) method combined with response surface methodology (RSM) was used for identification and optimization of factors influencing the extraction of aluminium from coal fly ash (CFA). The factors investigated included: acid concentration, leaching time, temperature and solid to liquid ratio. The significance of each factor and associated interactive effects were evaluated using a two-level factorial statistical design (2⁴) in conjunction with statistical software based on quadratic programming. Results showed temperature and time to be statistically significant; other factors and interactive effects were found to be insignificant. Optimization of the two significant factors was achieved by employing the second order quadratic regression model in combination with the central composite rotatable design (CCRD).

From the prediction model, an optimal aluminium extraction efficiency of 23.95% was obtained at optimal values of 82 °C temperature and 10.2 h leaching time. A confirmatory test showed an aluminium extraction efficiency of 24.8%, giving an error margin of 3.4%, with a linear correlation coefficient of 97.8%, hence verifying the fitness of the model and experimental data. The 24.8% extraction efficiency represents 89.3% aluminium extraction from the amorphous phase of CFA.

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VALIDITY OF CRITICAL COALESCENCE CONCENTRATION IN DYNAMIC CONDITIONS

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ABSTRACT

The aim of the study was to confirm that the concept of the critical coalescence concentration (Cho and Laskowski, 2002) is only applicable to static conditions.

A new experimental setup was developed. The experimental idea was to sample the same batch of bubbles at their formation point and later, during the bubble rise in static and dynamic conditions. The difference in the measured bubble size in the two sampling areas gives indication on the effect of frothers on bubble coalescence and breakup that takes place after the bubble creation due to the dynamic conditions.

Three commercial frothers, DF200, NF240 and DF250, were tested in the experiments.

In static conditions, the size of the forming and rising bubbles became equal at the frother concentration equal to the critical coalescence concentration (CCC) observed previously in mechanical flotation cell. On the other hand, in dynamic conditions, the size of rising bubbles was significantly larger than the size of freshly formed bubbles not only below the CCC as expected based on the literature. This finding confirms the hypothesis that the CCC is only applicable in static conditions, or in conditions where hydrodynamic forces do not contribute to bubble coalescence or breakup. The results showed that the frothers have a major effect on bubble size already at the early stage of bubble formation.

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THE USE OF DEXTRIN IN PURIFICATION BY FLOTATION OF MOLYBDENITE CONCENTRATES

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ABSTRACT

The process of flotation is commonly used for the recovery of molybdenite from mine tailings, but it produces low-content concentrates, thereby resulting in a product with low economic value. The low economic value is due to the presence of talc, which is a naturally hydrophobic mineral that is also floated with the molybdenite during the flotation process. Separability studies were conducted in a Partridge–Smith cell using dextrin as a molybdenite depressant in solution at different concentrations and pH values to produce a technical-grade concentrate (i.e., 90% MoS₂). These basic studies were accompanied by measurements of the zeta potential and contact angle, which was determined by the capillary rise method. The results of these floatability studies were used in bench tests of flotation, which were performed in a Denver D-12 cell. A molybdenite concentrate of 93.4% MoS₂ was obtained when dextrin was used at a concentration of 100 g/t.

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ENARGITE CONCENTRATE PROCESSING BY THE COMBINATION OF MECHANOCHEMICAL, HYDROMETALLURGICAL AND PRECIPITATION METHODS

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ABSTRACT

This paper investigates the possibility of enargite concentrate treatment using an environmentally friendly route. Enargite Cu_3AsS_4 contains dangerous arsenic, and this element can be removed by leaching with Na_2S in very alkaline environment ($\text{pH} > 12.5$). Arsenic passes into the leach, while the copper sulfide produced represents a raw material suitable for pyrometallurgy. We have shown that more than 80% of the arsenic can be extracted by atmospheric alkaline leaching at $95\text{ }^\circ\text{C}$, when mechanical pretreatment of enargite concentrate in an attritor is applied. The solubilized arsenic can be transformed into solid Na_3AsS_4 . The solid product Cu_2S can be further treated with elemental iron by mechanochemical reduction in a planetary mill. The final product forms a Cu/FeS composite from which iron can be separated by leaching with HCl . The proposed two-step process of milling (enhancement of arsenic removal (I) and obtaining of elemental copper (II)) illustrates the principal possibility of transforming minerals into metals.

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KINETICS AND MECHANISM OF SILICOTHERMIC REDUCTION PROCESS OF CALCINED DOLOMITE IN MAGNETHERM REACTOR

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ABSTRACT

The present study investigates the silicothermic reduction kinetic and mechanism of the dolomitic charges used in the magnetherm type reactors under inert atmosphere. The dolomitic charges are composed of a mixture of calcined dolomite (dolime) and ferrosilicon pressed in the briquettes form. Initially, these briquettes were sintered under argon at different temperatures 700–1000 °C, then reduced in magnetherm reactor. Different technical parameters such as the effect of sintering temperature, the reduction temperature (1450–1550 °C) and reduction time (up to 20 min) were investigated. The produced slag was characterized using XRD, XRF, and SEM techniques. Maximum reduction extent (about 80%) was achieved at optimum reduction conditions. These optimum conditions were double stoichiometric amount of silicon (2 ×) which is necessary to reduce all magnesium oxide present in dolomitic charges, sintering temperature of 700 °C for 1 hr, reduction time of 15 min and reduction temperature at 1550 °C. The results showed that the reduction of the dolomitic charge is controlled by the solid state diffusion process and the calculated value of the activation energy was found to be about 498 kJ/mol.

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SENSITIVITY OF PENTLANDITE FLOTATION IN COMPLEX SULFIDE ORES TOWARDS PH CONTROL BY LIME VERSUS SODA ASH: EFFECT ON ORE TYPE

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ABSTRACT

An extreme sensitivity of pentlandite flotation towards pH regulator at pH 10 has been documented using two types of complex nickel–copper sulfide ores in Northern Ontario, Canada. The samples studied are from Sudbury and Timmins areas and differ in their mafic and ultramafic associations and degree of dissemination. It has been shown that the pentlandite in the Timmins ore is completely depressed in the lime system at a collector dosage that readily floats the pentlandite in the Sudbury ore. The general mechanism of pentlandite depression by lime is believed to be similar to that of pyrite. However, the sensitivity of pentlandite in the Timmins ore is greatly affected by its ultramafic associations and is likely related to slime coating by serpentine minerals. The tenacity of hydrophilic calcium species in the case of the Sudbury ore is believed to be counteracted by a greater activation potential (e.g., level of Cu/Ni) and collector action. When lime is replaced by soda ash, adverse effect induced by adsorbed calcium species on pentlandite is largely eliminated. Benefit resulting from better dispersion of serpentinized species in the Timmins ore is also observed using soda ash. Chalcopyrite's strong floatability overcomes difficulties experienced by pentlandite and floats well both in the lime and soda ash systems. Pyrrhotite is less floatable than chalcopyrite and pentlandite in both lime and soda ash systems. In the lime system, pyrite depression is almost the same as pentlandite depression, but unlike pentlandite it continues to be non-floatable even in the soda ash system.

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SEPARATION OF MOLYBDENUM AND COBALT FROM SPENT CATALYST USING CYANEX 272 AND CYANEX 301

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ABSTRACT

Separation of molybdenum and cobalt from a spent catalyst leach liquor bearing 12.52 g/l Mo, 1.74 g/l Co and 9.98 g/l Al was investigated using solvent extraction technique followed by preparation of metal oxides. Cyanex 272 (bis(2,4,4-trimethylpentyl)phosphinic acid) and Cyanex 301 (bis(2,4,4-trimethylpentyl)dithiophosphinic acid) were used as extractants for molybdenum and cobalt, respectively. The effects of various parameters such as pH, concentration of extractant, A/O ratio and temperature on extraction of Mo and Co were studied. The number of stages required for extraction and stripping were determined from the McCabe–Thiele diagram and confirmed by counter current simulation study. The extracted species for Mo and Co were found to be $MoO_2A_2.H_2A_2$ and $CoA_2.H_2A_2$, respectively. The thermodynamic parameters such as ΔH , ΔS and ΔG were calculated for molybdenum and cobalt. The enthalpy change (ΔH) values for extraction of molybdenum and cobalt were positive indicating the extraction processes were endothermic. The oxides of molybdenum and cobalt were prepared from the strip solutions of molybdenum and cobalt by crystallization followed by thermal decomposition and the products were characterized by XRD and RAMAN spectra.

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AN OVERVIEW OF THE BENEFICIATION OF IRON ORES VIA REVERSE CATIONIC FLOTATION

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ABSTRACT

Flotation is the most effective solution, both technologically and economically, when upgrading iron concentrates. Research regarding iron ore flotation began in 1931, demonstrating that reverse cationic flotation is a very efficient method for beneficiating oxidised iron ores. This method can also be applied to reduce the silica content in magnetite concentrates obtained using wet low-intensity magnetic separation. Several studies describing the processing of iron ores via reverse cationic flotation are reviewed. The predominate role of the pulp mineralogy, as well as the type and molecular structures of the collectors and depressants, on flotation is discussed critically. The results concerning the role of the silicate mineralogy on the choice of reagents and flotation processes are also discussed. Further development of the reverse cationic flotation of iron ores requires a more detailed consideration of the nature of iron-bearing gangue minerals and the application of original approaches for the selective removal of these species.

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EXTRACTION OF LANTHANUM AND CERIUM FROM INDIAN RED MUD

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ABSTRACT

Laboratory-scale experiments were conducted to recover lanthanum and cerium from Indian red mud in sulfuric acid medium. The method includes acid leaching of red mud pulp and subsequent liquid–liquid extraction of the leached metals with different organic extractants, in order to establish the technical feasibility of extraction and separation simultaneously. Maximum recovery of lanthanum (99.9%) was recorded with 3 M H₂SO₄ at ambient (35 °C) temperature, S/L ratio of 10 g/L and agitation rate of 200 rpm in 1 h time. While 99.9% cerium recovery was achieved at 75 °C and solid/liquid ratio of 10 g/L in 3 M H₂SO₄. Significant specificity for complete extraction of lanthanum, cerium and scandium by Cyanex 301 was noted as compared to the solvents such as DEHPA and Cyanex 272.

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1. VISUALIZATION OF THE CONTROLLER STATES OF AN AUTOGENOUS MILL FROM TIME SERIES DATA

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ABSTRACT

The operational variables of an industrial autogenous mill were embedded in a low-dimensional phase space to facilitate visualization of the dynamic behavior of the mill. This was accomplished by use of a multivariate extension of the method of delay coordinates used in nonlinear time series analysis. In this phase space, the controlled states of the mill could be visualized as separate regions or clusters in the phase space. Comparison of the correlation dimension of the state variable of the mill (the load) embedded in phase space suggested that the dynamic behavior of the mill could not be represented by a linear stochastic model (Gaussian or otherwise). The low dimensionality (≤ 2) of the correlation dimension further suggested that the mill load depended on a few variables only and that the underlying generative process had a significant deterministic component. In addition, the operational variables could be used as reliable predictors in a neural network model to identify the controlled states of the mill. As a complementary approach to visualization of the operation of the mill, a different neural network model could be used to reconstruct a corrected power load curve by compensating for the effect of varying operating conditions.

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2. A CRITICAL REVIEW ON SOLVENT EXTRACTION OF RARE EARTHS FROM AQUEOUS SOLUTIONS

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ABSTRACT

Rare earth elements have unique physicochemical properties that make them essential elements in many high-tech components. Bastnesite (La, Ce)FCO₃, monazite, (Ce, La, Y, Th)PO₄, and xenotime, YPO₄, are the main commercial sources of rare earths. Rare earth minerals are usually beneficiated by flotation or gravity or magnetic processes to produce concentrates that are subsequently leached with aqueous inorganic acids, such as HCl, H₂SO₄, or HNO₃. After filtration or counter current decantation (CCD), solvent extraction is usually used to separate individual rare earths or produce mixed rare earth solutions or compounds. Rare earth producers follow similar principles and schemes when selecting specific solvent extraction routes. The use of cation exchangers, solvation extractants, and anion exchangers, for separating rare earths has been extensively studied. The choice of extractants and aqueous solutions is influenced by both cost considerations and requirements of technical performance. Commercially, D2EHPA, HEHEHP, Versatic 10, TBP, and Aliquat 336 have been widely used in rare earth solvent extraction processes. Up to hundreds of stages of mixers and settlers may be assembled together to achieve the necessary separations. This paper reviews the chemistry of different solvent extractants and typical configurations for rare earth separations.

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3. BIOLEACHING OF A LOW-GRADE COPPER ORE, LINKING LEACH CHEMISTRY AND MICROBIOLOGY

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ABSTRACT

Three largely-independent studies were undertaken on the same heap leach system during the period of transition from processing oxidised ores to sulfide ores: monitoring of heap solutions for microorganisms, analysis of samples from a spent heap, and column tests. Microbial cell numbers and diversity were monitored in process water samples from the transition heap over a four-year period. Cell numbers remained low throughout, $1\text{--}30 \times 10^4$ cells mL⁻¹, possibly reflecting growth inhibition by the high element concentrations in process water. High iron, magnesium and aluminium concentrations in spent heap pregnant leach solution (PLS) are attributed to siderite and clinocllore dissolution and would be expected to impact on microbial growth. Planktonic cell numbers in a column leachate declined rapidly by two orders of magnitude when concentrations of ferric ion and sulfate exceeded 30 and 75 g L⁻¹, respectively. Nevertheless, a variety of bacterial strains closely related to *Acidithiobacillus* (*At.*) *ferrooxidans*, *At. caldus*, *Leptospirillum* (*L.*) *ferriphilum*, *Acidimicrobium* (*Am.*) *ferrooxidans*, *Acidiphilium* (*Ap.*) *cryptum*, an *Alicyclobacillus*-related strain and *Sulfobacillus* (*S.*) *thermosulfidooxidans*, and the archaeon *Ferroplasma* (*F.*) *acidiphilum* were isolated, mainly from the more acidic intermediate leach solutions (ILS). Overall, the results obtained from the use of culture-dependent and culture-independent methods of community analysis were complementary and consistent. The majority of identified genera and species were present in both the process water samples from the operating heap and the solutions and ore samples from the spent heap. In the spent heap, distinct populations dominated different sample types. *Leptospirillum*- and *Acidithiobacillus*-like strains dominated PLS samples and *Leptospirillum* also dominated seven of eight spent ore samples and all of the heap sediment samples, making it the primary iron(II) oxidising species.

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4. EFFECTS OF SLURRY FILLING AND MILL SPEED ON THE NET POWER DRAW OF A TUMBLING BALL MILL

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ABSTRACT

The pool of slurry is known to lower the power drawn to the mill. An attempt to ascertain this observation by relating load orientation to mill power for a range of speeds and slurry fillings was undertaken. To this end, a Platinum ore ($-850\ \mu\text{m}$) was used to prepare a slurry at 65% solids concentration by mass. The Wits pilot mill ($552 \times 400\ \text{mm}$), initially loaded with 10 mm balls at 20% volumetric filling, was run at 5 different speeds between 65% and 85% of critical. The net power draw and media charge position were measured. After this, the slurried ore was gradually added to the media charge for slurry filling U between 0 and 3. A proximity probe and a conductivity sensor mounted on the mill shell provided a means of measuring both the position of the media charge and that of slurry. The data collected for the load behaviour and net power draw was later analysed. It was found that Morrell's model could not fully explain the effect of slurry volume on net power draw especially for an under-filled media charge (i.e., for $U < 1$). The size of lifters and grinding balls used could be the reason for this. That is why a piece-wise function was curve-fitted to the power data to help make sense of the inconsistencies observed.

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5. AN INNOVATIVE PROCESS FOR EXTRACTING BORON AND SIMULTANEOUS RECOVERING METALLIC IRON FROM LUDWIGITE ORE

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ABSTRACT

Ludwigite ore has not yet been utilized on an industrial scale due to its complex mineralogy and fine mineral dissemination in China. Boron–iron separation and dissolution activity of boron-bearing minerals in alkaline liquor are the two key issues in the utilization of ludwigite ore, governing the boron recovery as well as operating cost. This paper proposes an innovative process for extraction of boron and iron from ludwigite ore based on coal-based direct reduction process with sodium carbonate (Na_2CO_3). The novel process involves reduction roasting, combined leaching and grinding of reduced ludwigite ore, followed by magnetic separation of leach residue, and experimental validation for each of the processing steps is demonstrated. Alkali-activation of boron and metallization of iron were synchronously achieved during carbothermic reduction of ludwigite ore in the presence of Na_2CO_3 . Consequently, boron was readily extracted in the form of sodium metaborate (NaBO_2) with water at room temperature during ball mill grinding, and metallic iron powder was recovered from the leaching-filtering residue by magnetic separation. Boron extraction of 72.1% and iron recovery of 95.7% with corresponding iron grade of 95.7% in the magnetic concentrate were achieved when ludwigite ore was reduced with 20% sodium carbonate at 1050 °C for 60 min.

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6. VEGETATION RESPONSE OF AUSTRALIAN NATIVE GRASS SPECIES REDGRASS (*BOTHRIOCHLOA MACRA* (STEUDEL) S.T. BLAKE) AND SPIDER GRASS (*ENTEROPOGON ACICULARIS* (LINDL.) LAZARIDES) IN SALINE AND ARSENIC CONTAMINATED GOLD MINE TAILINGS: A GLASSHOUSE STUDY

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ABSTRACT

The stabilization of sulphidic wastes produced by underground gold mining is challenging because these materials are often structureless, saline and contain elevated levels of toxic metalloids. A glasshouse study was conducted to test a milled benign waste rock and topsoil. The test species were, *Bothriochloa macra* (Steud) S.T. Blake and *Enteropogon acicularis* (Lindl.) Lazarides, two warm season drought-tolerant native grasses from Australia with the potential to be used for phytostabilization. Rhizocylinders were used in order to examine root structures for plants grown in the various treatments. Soil water samples were also extracted from the various substrates and analyzed for soluble arsenic (As), along with pH, electrical conductivity and redox potential. Growth trials were carried out for 100 days. Growth indices, including biomass accumulation, leaf area, root:shoot ratio and chlorophyll fluorescence were measured along with relative growth rate (RGR) calculations. Results showed a significant decrease in growth across all growth indices for grasses grown on mine tailings. An oxidized waste rock layer and topsoil exhibited high growth, especially for the species *E. acicularis*. Small amounts of As were detected in the leaf tissue of *B. macra* and *E. acicularis* after growth in As contaminated substrates, but it was found that As levels in plant tissue did not correlate with As levels in the soil water. These grasses did not readily accumulate As, and it is highly unlikely that any As contained in the grass material will biomagnified through the food chain or increase environmental pollution from mine sites. Substrate analysis found the highest bioavailable levels of As occurred in the crushed oxidized rock matrix. However, when compared to growth results, this substrate supported significantly high growth.

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7. MINE OPERATING COSTS AND THE POTENTIAL IMPACTS OF ENERGY AND GRINDING

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ABSTRACT

An understanding of the breakdown of mine costs is an important tool for researchers and developers who seek to place novel cost-reducing unit operations in the wider general cost context. This paper provides a breakdown of operating costs in 63 mines by dividing them into three main categories: mining, milling, and general and administrative (G & A) costs. The study looks at patterns in mining type, mill processing type, mineral type, and the differences between costs expressed in feasibility studies vs. operating mines. The paper explores the reasons for the relationships observed and then presents a total average mine cost breakdown. It was found that the mean relative mining and milling costs did not differ significantly, and that on average they had equal shares of the total enterprise operating costs. Effects of mine and mineral type were observed, with underground milling costs being significantly less than open pit milling costs and gold mines occupying a significantly larger share of mine operating costs than copper-containing mines. The overall relative operating costs were found to be in the ratios between (43:43:14) and (45:45:10) (Mine:Mill:G & A). A treatment of potential unit operations and innovative technologies is provided at the conclusion of the paper, including coarse particle recovery by flotation and novel grinding technologies.

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8. CONTROL ORIENTED MODELING OF FLOW AND SIZE DISTRIBUTION IN CONE CRUSHERS

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ABSTRACT

This work presents a dynamic model for prediction of flow and output size distribution of cone crushers. The main purpose of the model is for simulation of closed-loop control using the Closed Side Setting (CSS) and the eccentric speed (ω) as manipulated variables. The idea of modeling crushers as cascaded zones is adopted throughout this work. The capacity, the length, the stroke, and the compression ratio of each zone are taken into consideration. Simulation results are presented in the form of the Crusher Performance Map (CPM) and the dynamic response for production of different size classes to steps input in ω and CSS. The simulations also include operation with recycling of oversize output, as well as the input of mixed materials. As an example, closed-loop control of the ratio of the large-size output to the total size output was simulated.

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9. PREDICTION OF WEAR AND ITS EFFECT ON THE MULTIPHASE FLOW AND SEPARATION PERFORMANCE OF DENSE MEDIUM CYCLONE

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ABSTRACT

Modern coal preparation plants. It is known that wear is one of the problems in the operation of DMCs, but it is not well understood. In this work, the wear rate of DMC walls due to the impact of coal particles is predicted by a combined computational fluid dynamics and discrete element method (CFD-DEM) approach, using the Finnie wear model from the literature. In the CFD-DEM model, DEM is used to model the motion of discrete coal particles by applying Newton's laws of motion and CFD is used to model the motion of the slurry medium by numerically solving the local-averaged Navier–Stokes equations together with the volume of fluid (VOF) and mixture multiphase flow models. Dense medium cyclone (DMC) is a high-tonnage device that is widely used to upgrade run-of-mine coal in According to the Finnie wear model, the wear rate is calculated according to the impact angle of particles on the wall, particle velocity during an impact and the yield stress of wall material; the relevant particle-scale information can be readily obtained from the CFD-DEM simulation. The numerical results show that the severe wear locations are generally the inside wall of the spigot and the outside wall of the vortex finder. The wear rate depends on both the operational conditions and solids properties. It increases generally with the decrease of medium-to-coal (M:C) ratio. For a given constant M:C ratio, the wear rate for thermal coal is higher than that for coking coal, especially at the spigot. Large particles may cause a non-symmetric wear rate due to the gravity effect. The effect of a worn spigot wall on the multiphase flow and separation performance is also studied. This work suggests that the proposed approach could be a useful tool to study the effect of wear in DMCs under different conditions.

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10. CFD MODELLING OF FLUID FLOW IN A PEIRCE–SMITH CONVERTER WITH MORE THAN ONE INJECTION POINT

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ABSTRACT

Copper converting is mainly conducted in Peirce–Smith converters. Extensive work has been conducted to understand fluid flow phenomena as air is injected into molten mattes. High momentum must be transferred from the gas to the melt in order to refine the metal. In this work, we present a CFD analysis of gas injection with one and three tuyeres. Results show that by increasing the number of injection points, the flow pattern within the converter change considerably. Such changes result in the development of large recirculation zones and localised eddy formation. Additionally, it was found that the gas plumes in the melt are asymmetrical thus flow paths constantly interfere between themselves. Bubbling–jetting transition is found to be better represented by the Kutateladze number.

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11. THE APPLICATION OF WOOD ASH AS A REAGENT IN ACID MINE DRAINAGE TREATMENT

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ABSTRACT

The paper deals with a possible utilisation of wood ash as a reagent in treating acid mine drainage (AMD) from opencast mining of brown coal. Wood ash samples were obtained having combusted deciduous and coniferous tree wood in a household furnace. The dominant mineral phases in wood ash are calcite, quartz, lime and periclase. The used AMD is characteristic of high contents of sulphates, iron, manganese, heavy metals and low pH. The AMD treatment process included dosing of wood ash to adjust pH values about 8.3 (a dose of 0.5 g l^{-1}) or calcium hydroxide (a dose of 0.2 g l^{-1}) for comparison. The reaction time was 20 min. Dosing of wood ash in AMD resulted in an increase of pH in solution from 3.5 to 8.3, which caused the removal of metal ions mainly by precipitation, co-precipitation and adsorption. Comparing the application of $\text{Ca}(\text{OH})_2$ in AMD treatment, at an almost identical pH value the concentrations fell in both cases for Fe, Mn, As, Co, Cu, Ni, Zn, Mg, Al and Mo. Applying wood ash the drop was even more distinct in Mn, Zn and Mg. The results of sedimentation tests in an Imhoff cone confirm that the settling capacities of sludge using wood ash are significantly better than when using calcium hydroxide in acid mine drainage treatment.

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12. CHARACTERISATION AND LIBERATION OF CHROMIUM FROM FINE FERROCHROME WASTE MATERIALS

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ABSTRACT

Three types of generic chromium (Cr)-containing wastes are generated during ferrochrome (FeCr) production, i.e. slag, bag filter dust (BFD) and venturi sludge. Slag is by volume the largest waste; however, fine FeCr waste materials (e.g. BFD, venturi sludge) are from an environmental perspective the most important. The loss of Cr units to FeCr waste streams represents both an added cost burden (related to disposal/storage) and a loss of revenue in terms of contained Cr units. In this paper, the novel idea of the liberation of Cr units from FeCr BFD and the ultra-fine fraction of slag (UFS) with aqueous ozonation and the advanced oxidation process was investigated. Several techniques were used to characterise both case study waste materials, i.e. particle size distribution, chemical composition, chemical surface composition and crystalline content analysis. Results indicated that limited Cr liberation could be obtained from the waste materials utilising aqueous ozonation. For BFD, only a maximum of 4.2% of total Cr liberation was achieved. However, the Cr liberation of BFD was substantially higher than that achieved for the UFS, which was attributed to the difference in characteristics of the two materials. Cr liberation observed was related to the formation of the OH[·] radicals during the spontaneous decomposition of aqueous O₃. Application of the advanced oxidation process by the addition of H₂O₂ during ozonation increased Cr liberation dramatically. More than 21% of total Cr liberation could be achieved for both the waste materials used in this investigation. Although the afore-mentioned Cr liberation level is unlikely to be commercially viable, the investigation proved that further research could optimise this process.

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13. DETERMINING FROTHER-LIKE PROPERTIES OF PROCESS WATER IN BITUMEN FLOTATION

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ABSTRACT

In oil sands flotation, bitumen is known to release natural surfactants into the process water following the addition of NaOH. These surfactants appear to replace the need for frother. Measuring the Sauter mean diameter (D_{32}) vs. dilution, it was possible to characterize the frother-like properties of process waters as an equivalent concentration of a known frother commonly used in mineral flotation, DF-250. Process water samples from the thickener overflow at the Shell Albian plant were examined. The study showed equivalent concentrations up to 60 ppm DF-250 and variations between samples. Reasons for the variability are discussed. A gas holdup vs. D_{32} correlation was established which reduced the experimental effort.

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14. THE APPLICABILITY OF THE KUBELKA–MUNK MODEL IN GCC BRIGHTNESS PREDICTION

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ABSTRACT

Ground calcium carbonate (GCC) is one of the most commonly used pigments in paper. In order to study the colouring effect of selected minerals on a GCC slurry, a high-quality calcite concentrate was spiked with contaminating minerals prior to micronisation and subsequent spectrophotometric measurements. 14 different mineral contaminant concentrates were tested: pyrite, pyrrhotite, chalcopyrite, galena, sphalerite (light and dark type), magnetite, hematite, ilmenite, quartz, K-feldspar, phlogopite, hornblende and graphite. The results show that the pyrrhotite, chalcopyrite and graphite concentrates display the most detrimental reduction in brightness R457 of the GCC slurry. In addition to brightness, the colour space for each contaminant concentrate is evaluated by using the CIELAB parameters. Furthermore, by applying the Kubelka–Munk function, the results show that most of the contaminants tested follow the Kubelka–Munk model with good accuracy, allowing a prediction of the brightness in a mixture to be made. Hence, the Kubelka–Munk model can provide a useful method to predict the colour of mineral mixtures in the production of GCC slurries.

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15. DECOUPLING RHEOLOGY AND SLIME COATINGS EFFECT ON THE NATURAL FLOTABILITY OF CHALCOPYRITE IN A CLAY-RICH FLOTATION PULP

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ABSTRACT

Clay minerals are a commonly occurring gangue in mineral beneficiation operations and occur in a variety of ore deposits, including porphyry copper ores. The presence of clays in mineral beneficiation circuits can cause a wide range of different problems, including that of slime coatings on valuable minerals and elevated viscosities of flotation pulps. The aim of this work was to decouple and estimate the relative magnitudes of the slime coatings and pulp rheology effects on the natural floatability of chalcopyrite in a model mineral system. It was found that the two phenomena can be partially isolated and that they both have a detrimental effect on flotation performance. It was also found that the level to which these two phenomena affect chalcopyrite recovery is of a similar order of magnitude.

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16. GEMINI TRISILOXANE SURFACTANT: SYNTHESIS AND FLOTATION OF ALUMINOSILICATE MINERALS

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ABSTRACT

In this paper, an amino-trisiloxane Gemini cationic surfactant, butane-1,4-bis(dimethyl-(3-(3-aminopropyl trisiloxane-3-yl)-propyl)-ammonium bromide) (BBAB) was prepared, and its flotation potential was assessed on kaolinite, pyrophyllite and illite minerals. The flotation results showed that changes to the pulp pH did not significantly influence BBAB's collecting power in floating three aluminosilicate minerals. In addition, BBAB was a stronger collector than the conventional monomeric surfactant dedecyl trimethylammonium bromide (DTAB) or dodecylamine (DDA). The results of FTIR spectra, zeta potential measurements and density functional theory (DFT) calculations indicated that the interaction of BBAB with the three aluminosilicates was mainly through electrostatic attraction. BBAB's unique properties, such as high positive grouping Mulliken charge of $-\text{CH}_2\text{N}^+(\text{CH}_3)_2(\text{CH}_2)_4(\text{CH}_3)_2\text{N}^+\text{CH}_2-$, and "parachute" shape structure of $[(\text{CH}_3)_3\text{SiO}]_2\text{SiCH}_3$, resulted in superior collecting powers for the aluminosilicate minerals.

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17. LITHIUM EXTRACTION FROM B-SPODUMENE THROUGH CHLORINATION WITH CHLORINE GAS

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ABSTRACT

The extraction of lithium by means of the chlorination roasting of β -spodumene has been studied in the temperature range from 1000 to 1100 °C for periods of time from 0 to 180 min. The roasting was carried out in a fixed bed reactor using pure gaseous Cl_2 as chlorinating agent. The reactants and products were characterized by X-ray diffraction (XRD), X-ray fluorescence (XRF), atomic absorption spectrometry (AAS), scanning electron microscopy (SEM) and electron probe microanalysis (EPMA). The roasting of β -spodumene with pure Cl_2 at 1100 °C for the period of 150 min led to quantitative extraction of lithium as lithium chloride. The solid products of the reaction of β -spodumene with Cl_2 were found to be $\text{Al}_6\text{Si}_2\text{O}_{13}$ (mullite), and Si_2O (cristobalite).

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1. TOF-SIMS STUDIES OF SURFACE CHEMISTRY OF MINERALS SUBJECTED TO FLOTATION SEPARATION – A REVIEW

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ABSTRACT

This paper reviews the applications of time of flight secondary ion mass spectrometry (TOF-SIMS) used for surface chemical analysis of mineral in the context of froth flotation. A wide range of applications are reviewed, including; interactions of reagents on the surface of mineral phases during flotation separation, determining the effects of various transferred ions from different minerals or the slurry, evaluation of hydrophobicity, identifying the relationship between mineral surface chemistry and contact angle, and evaluation of grinding effects. Conclusions indicated that TOF-SIMS, as a unique surface analysis technique, can potentially provide a direct determination of parameters which control the surface reactivity and consequently plays an important role in determining flotation behaviour of minerals.

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2. GAS DISPERSION MEASUREMENTS IN MECHANICAL FLOTATION CELLS: INDUSTRIAL EXPERIENCE IN CHILEAN CONCENTRATORS

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ABSTRACT

This technical note presents results of gas dispersion measurements carried out in industrial mechanical flotation cells from Chilean concentrators. Results showed that superficial gas rate, gas holdup and bubble size were within ranges found in literature. The bubble surface area fluxes (S_B) were computed using the superficial gas rates and the Sauter mean diameters, obtaining approximate S_B ranges from 20 m²/s/m² to 60 m²/s/m² for both self-aerated and forced-air flotation cells. Despite the different cell types, sizes and wide range of operating conditions, an exponential relationship between superficial gas rate (J_G) and Sauter mean diameter (D_{32}) was obtained:

$$D_{32} = D_0 \cdot e^{\gamma J_G}, D_0 = 0.77 \pm 0.11, \gamma = 0.77 \pm 0.09$$

This result allows predicting D_{32} as a function of J_G . Data on gas holdup (ϵ_G) as a function of Sauter mean diameter were also presented: For $J_G < 1.2$ cm/s, gas holdup increases as superficial gas rate increases, indicating a dominant effect of superficial gas rate; for $J_G > 1.2$ cm/s, gas holdup decreases as D_{32} increases, indicating a predominant effect of bubble coalescence.

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3. ELECTROCHEMICAL ENHANCED OXIDATIVE DECOMPOSITION OF CHROMITE ORE IN HIGHLY CONCENTRATED KOH SOLUTION

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ABSTRACT

A novel method which introduces an electrochemical field to enhance the oxidative decomposition of chromite in a KOH sub-molten salt medium was proposed and proven to be feasible and efficient. Under optimal reaction conditions (slot current density 750 A/m², alkali concentration 60 wt.%, reaction temperature 150 °C, alkali-to-ore mass ratio 6:1, and particle size <200 mesh), the extraction rate of chromium reached 99%, after reacting for 480 min. In comparison with the current liquid-phase oxidation technologies, the reaction temperature in the new approach is 150–250 °C lower, and the alkali concentration of the reaction medium is lower by more than 20%, showing substantial advantages in terms of energy efficiency, equipment corrosion alleviation and prospects for industrial application. The reaction kinetics study shows that the extraction process under optimal reaction conditions is jointly governed by surface chemical reaction and solid product layer diffusion with the apparent activation energy calculated to be 17.56 kJ/mol.

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4. LEACHING BEHAVIOUR OF NATURAL AND HEAT-TREATED BRANNERITE-CONTAINING URANIUM ORES IN SULPHATE SOLUTIONS WITH IRON (III)

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ABSTRACT

Uranium leaching tests were conducted on two naturally occurring, highly metamict brannerite ores from the Crockers Well and Roxby Downs deposits, South Australia. The ores were leached over a range of temperatures and Fe^(III) and H₂SO₄ concentrations. As well, samples of the ores were calcined at 1200 °C in air to investigate the effect of thermally induced recrystallisation on uranium dissolution. For the unheated samples, a maximum of ~80% U dissolution was obtained using an Fe^(III) concentration of 12 g/L, an acid concentration of 150 g/L H₂SO₄ and a temperature of 95 °C. The heat treated samples performed poorly under identical conditions, with maximum uranium dissolution of <10% recorded. High uranium dissolution from natural brannerite can be achieved providing; (i) acid strength, oxidant strength and temperatures are maintained at elevated levels (compared to those traditionally used for uraninite leaching), and, (ii) the brannerite has not undergone any significant recrystallisation (e.g. through metamorphism).

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5. DIETHYLENETRIAMINE DEPRESSION OF CU-ACTIVATED PYRITE HYDROPHOBISED BY XANTHATE

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ABSTRACT

In copper sulphide flotation, copper adsorbs on pyrite through superficial oxidation of the copper minerals (e.g. chalcopyrite) which promotes pyrite flotation in the presence of xanthate. This “inadvertent” activation of pyrite by copper ions is undesirable in copper sulphide flotation. In order to minimise this effect, depressants are used to suppress the effect of the activating ions. The effect of diethylenetriamine (DETA) in different combinations (under aerated and non-aerated conditions) on Cu-activated pyrite hydrophobised by xanthate was examined using flotation, spectroscopic and solution analyses, at pH 10. The results showed that DETA affects the flotation behaviour and surface chemistry of pyrite. However, high dosages are required. The depression action of DETA on Cu-activated pyrite was attributed to both the removal of surface copper to form soluble Cu-DETA complex in solution and competition for Cu sites on the activated pyrite surface. The significant depression of pyrite in the presence of DETA under the aerated condition was due to increased amount of iron oxy-hydroxides (Fe-O/OH), copper oxides and Cu(I)-DETA hydrophilic species.

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6. INFLUENCE OF THE PROPAGATION OF THREE PHASE CONTACT LINE ON FLOTATION RECOVERY

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ABSTRACT

Froth flotation is considered the most effective process of beneficiating low grade ores and is widely used in the base metals industry. For effective flotation, the attachment of mineral particles to air bubbles is important and has been studied by many researchers by measuring quantities such as attachment time, film-thinning time and induction time. This paper identifies an important step in the bubble-particle attachment process, namely, the expansion mechanism of the three phase contact (TPC) line between liquid, solid and air. It has been shown that the TPC expansion time is determined by the drainage of the surrounding fluid. It is influenced by factors such as pulp chemistry surrounding the particle, variations in surface forces and pressure inside the bubble. It has been observed experimentally that the TPC expansion time bears square root relationship to attachment efficiency. In this work, it has been argued that the attachment efficiency is related to the TPC circle radius propagation.

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7. EFFECT OF VORTEX FINDER DIAMETER ON THE PERFORMANCE OF A NOVEL HYDROCYCLONE SEPARATOR

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ABSTRACT

Hydrocyclones are equipments widely used by the mineral industry, but it is possible to highlight its operation in desliming, selective classification, thickening and pre-concentration. Our research group designed a new hydrocyclone. In this novel device, the conical section of a conventional hydrocyclone was replaced by a conical filtering wall and the equipment was named filtering hydrocyclone. During the operation of this novel hydrocyclone, besides the underflow and overflow streams, there is another stream of liquid, resulting from the filtrate produced in the porous cone. In the present work, the influence of vortex finder diameter (D_o) of a filtering hydrocyclone was analyzed by an experimental and CFD study. Data from a conventional hydrocyclone of the same configuration were also obtained. The results indicated that the performance of separation process was significantly improved with this new equipment. Depending on the specific functions of the separator (as a classifier or thickener) the best values of D_o were also found for the filtering hydrocyclone.

8. PREDICTING PLANT SCALE FLASH FLOTATION PERFORMANCE – VALIDATION OF LABORATORY METHODOLOGY AND APPLICATIONS FOR USE

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ABSTRACT

A method has been developed in which laboratory batch flotation test results can be used in conjunction with mineralogical analysis to determine whether an ore is amenable to successful recovery via the flash flotation processing route. In the original development work, using a high grade refractory gold ore, a direct correlation was found with the particle properties of the plant flash flotation cell concentrate and a concentrate produced by a targeted laboratory batch flotation test. The respective concentrates were observed to have nearly identical distributions of the target elements (Au, S and Fe) by size as well as almost identical liberation characteristics of the key mineral (pyrite) for flotation. A second ore from the same mine, but of significantly lower grade and different grinding characteristics has now been tested to determine if the same correlations exist that were observed with the previous work and to provide further insight into the differences between laboratory and plant response in order to potentially refine the procedure further and enhance its usability as a predictive tool.

Testing of the second ore confirmed the original findings that a targeted laboratory batch flotation test can produce a concentrate with a target mineral (pyrite) distribution by size and liberation that matches the concentrate produced by the industrial scale flash flotation cell whilst treating the same feed material. Further to this, grades of the intermediate size classes in the laboratory concentrates were found to be similar to those of the plant flash cleaner cells.

From the correlations in performance observed with both ore types in the laboratory batch cell and plant flash flotation cell, methodologies are proposed that can be used to determine:

- whether a new ore could be treated by flash flotation in a plant with an existing flash flotation circuit;
- whether a plant operating without an existing flash flotation circuit could benefit from installing one; and
- the amenability of an ore to the flash flotation process for greenfield flow sheet development.

A step wise approach is given for each to allow the method to be applied to and adapted for other ores and valuable mineral types. The advantage of following this methodology exists in that no specialised equipment or analysis methods are required to perform the test. Standard laboratory equipment has been used throughout the test-work and mineralogical

analysis performed via commercially available MLA. The procedure is kept as basic as possible to allow for maximum usability on sites where only essential laboratory equipment exists.

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9. KIMBERLITE WEATHERING: EFFECTS OF ORGANIC REAGENTS

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ABSTRACT

Kimberlite material is one of the primary sources of diamonds. Accelerated weathering that leads to a physical breakdown of the material over a short period of time has possible benefits in diamond processing such as reduction in the energy consumption when used as a pre-comminution stage. This study investigated accelerated weathering by utilising organic reagents; acetic acid, ethanol, formamide, n-hexane, oxalic acid, and urea, in comparison to the use of Cu^{2+} solution that was previously shown to be very effective in weathering kimberlite. Oxalic acid was the organic agent that showed promising weathering capabilities. However, the use of organic solutions was not as efficient as with Cu^{2+} solutions. Results showed that 67% of the particles passed 12 mm screen size in Cu^{2+} weathering compared to 48% in oxalic acid. It was also found that time of exposure had a small effect on weathering. Increasing the organic chemical concentration twofold, from 0.025 M to 0.5 M, improved weathering by ~20% points. Different weathering mechanisms were observed at different solution concentration between oxalic acid (1st to 2nd order) and Cu^{2+} (2nd to 3rd order).

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10. FROTH FLOTATION OF SPHALERITE: COLLECTOR CONCENTRATION, GAS DISPERSION AND PARTICLE SIZE EFFECTS

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ABSTRACT

This experimental work on sphalerite flotation investigated the effect on flotation performance of three particle size fractions, namely, coarse ($d_{80} = 100 \mu\text{m}$), medium ($d_{80} = 39 \mu\text{m}$) and fine ($d_{80} = 15 \mu\text{m}$), bubble size distribution, superficial air velocity, and collector dosage. Bubble size distributions were characterized with the image analysis technique. The two-phase (liquid–gas) centrifugal pump and frother addition (MIBC, 5–30 ppm) allowed generating bubble diameters between 150 and 1050 μm , and air holdup ranging from 0.2% and 1.3%. Main results showed that each particle-size distribution required an optimal bubble-size profile, and that sphalerite recovery proceeded from mechanisms involving true flotation (when $J_g = 0.04 \text{ cm/s}$ and $1.9 \times 10^{-4} \text{ M SIPX}$). However, cluster-flotation occurs at high collector dosage (when $J_g = 0.04 \text{ cm/s}$ and d_{32} between 285 and 1030 μm), and requiring further investigation.

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11. ELECTRICAL DISINTEGRATION AND MICRO-FOCUS X-RAY CT OBSERVATIONS OF CEMENT PASTE SAMPLES WITH DISPERSED MINERAL PARTICLES

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ABSTRACT

Electrical disintegration is an effective liberation technique in mineral processing where the liberation ratio depends on the mineralogical properties of the mineral grains. However elucidation of the liberation behavior is difficult since the fragments after the electrical disintegration are fine and complex. This study applies electrical disintegration to cement paste samples with various dispersed mineral particles (calcite, quartz, albite, and pyrite) and the disintegrated products are observed with a micro-focus X-ray CT scanner. Current channels and crack extension behavior from the channels are identified by cross sectional CT and three dimensional reconstructed images. A classification of the crack patterns was carried out and compared with the results of liberation ratio measurements of the products.

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