Process Safety and Environmental Protection

Rok 2019, Volume 121

January

Auchitya Verma, Subrata Hait. *Chelating extraction of metals from e-waste using diethylene triamine pentaacetic acid*. Pages 1-11.

In this study, the chelating extraction of base metals namely, Cu, Zn, Ni from printed circuit board (PCB) of obsolete computer was carried out using diethylene triamine pentaacetic acid (DTPA) as a safer ligand. At a liquid to solid ratio (L/S ratio) of 50 and the comminuted PCB in the size range of 0.038–1 mm, the maximum extraction of around 97% Cu at 4.5 d and more than 99% each of Zn and Ni at 3 d was achieved using 0.5 M DTPA at pH of 9, temperature of 50 °C and mixing speed of 450 rpm. Using 0.9 M H2O2 under optimized process conditions, around 99% Cu and 82% Ni leaching were achieved in 8 h along with complete leaching of Zn in 1 h only. Kinetics development using the shrinking core model (SCM) indicated that the metal extraction from the PCB comminution fines using DTPA is controlled by diffusion process. Further, metal recovery of around 98% each for Cu and Ni and 95% for Zn was achieved by the chemical precipitation of the leachate. Chelating extraction using DTPA coupled with the chemical precipitation of the leachate has the potential to emerge as a complete solution for metal recycling from e-waste.

- **Keywords:** E-waste; Printed circuit board; Metals; Chemical leaching; Chelation; DTPA

E.G. de Moraes, M. Bigi, N.P. Stochero, S. Arcaro, C. Siligardi, A.P. Novaes de Oliveira. *Vitrocrystalline foams produced with EPS as pore former: Processing and characterization*. Pages 12-19.

In this work, discarded soda-lime-silica glasses (from glass bottles) and expandable Styrofoam, EPS (d50 < 1 mm) were successfully converted into vitrocrystalline foams for thermal insulation applications. Physical, chemical and thermal properties of the selected and prepared raw materials (wastes) were characterized. Batches containing well mixed glass powder (d50 < 5 μm), EPS powder beads (10–40 vol.%) and Bonder Plus® (Na2SiO3 solution) were prepared so that powder compacts uniaxially pressed at 20 MPa were obtained. The powder compacts were dried at room temperature for 24 h and then fired at 850 °C, 10 °C/min for 30 min. Vitrocrystalline foams with interconnected cells sizes between 150 and 850 μm, homogeneously distributed in a crack free matrix were produced and characterized from the point of view of their typical physical, chemical, morphological, thermal conductivity and mechanical properties. The results showed that it is possible to obtain vitrocrystalline foams (cristobalite and devitrite as crystalline phases), with porosity up to 90%, compressive strength of 2.75 MPa and thermal

conductibility of 0.06 W/m K, for foams containing 40 vol% of pore former. The magnitude of the measured properties of the produced vitrocrystalline foams are adequate for a number of applications requiring low thermal conductivity.

- **Keywords:** Vitrocrystalline foams; Bottle glasses; Styrofoam; Pore forming agents; Thermal insulation

Philip Isaac Omwene, Meltem Çelen, Mehmet Salim Öncel, Mehmet Kobya. *Arsenic removal from naturally arsenic contaminated ground water by packed-bed electrocoagulator using Al and Fe scrap anodes*. Pages 20-31.

In this work, feasibility of electrocoagulation (EC) process with Al and Fe scrap anodes for treatment of groundwater contaminated with arsenic (As) was examined as a cheaper treatment alternative for affected remote communities. EC experiments were carried out in a batch packed-bed EC reactor and the effect of applied current (0.010–0.100 A), type of scrap electrode (Fe and Al), packed-bed density (0.1–0.4 kg/m3 for Fe and 0.02–0.08 kg/m3 for Al) and EC time were investigated. Optimum operating conditions to obtain maximum contaminant level (MCL) of 10 μg /L for total As (>93% removal) in groundwater samples were determined as 8 min and 0.05 A for Fe scrap anodes. Whereas for Al scrap anode, 30 min and 0.10 A were the optimums. The operating cost, energy and electrode consumptions at these optimums were calculated as 0.017 US $/m3, 0.070 kW h/m3 and 0.052 kg/m3 for Fe anodes and 0.181 US $/m3, 0.876 kW h/m3 and 0.067 kg/m3 for AL anodes respectively. The As removal slightly decreased with decrease in anode bed density. Moreover, Fe scrap anodes exhibited better As removal than the Al scrap anodes at all tested conditions. The scanning electron microscopy (SEM) of the electro-coagulated sludge revealed irregular and porous particles with amorphous structure. The Fourier-transform infrared spectroscopy (FTIR) showed bonding between Fe(III) - As(V), and AsO bond, confirming As removal by co-precipitation and adsorption, respectively in the EC process.

- **Keywords:** Arsenic; Electrocoagulation; Al and Fe scrap anodes; Groundwater

Fan Geng, Changgeng Gui, Yingchao Wang, Fubao Zhou, Shengyong Hu, Gang Luo. *Dust distribution and control in a coal roadway driven by an air curtain system: A numerical study*. Pages 32-42.

Dust pollution is one of the most serious problems in underground coal mines. To effectively control dust, it is necessary to investigate the dust distribution in the coal roadways. In this study, the dust distribution under the isolation effect of an air curtain was investigated in a coal roadway. First, the coal roadway was presented with a vault, a hybrid ventilation system, and an air curtain system installed on the digging machine. Second, the dust movement was simulated via the Euler-Lagrange method. Meanwhile, dust was treated as a discrete phase under a Lagrangian frame, and the air flow was modelled as the continuous phase. Then the spatiotemporal distribution of dust in the coal roadway was studied with and without the air curtain system. The results show that the spatiotemporal concentration of dust clearly reduces after the air curtain when compared with that of the system without the air curtain and the conventional hybrid ventilation system (FSNE), particularly for the working area. The isolation action of the air curtain is obvious for total dust. It is also found that the air curtain system can obviously reduce the dust concentration on the side of the operator, and provide a cleaner environment for the miners. Moreover, selected results show agreement with the relevant experimental and simulation ones. The air curtain is useful for resolving the problem of dust-isolation in the coal roadway, and can be used to improve the working environment in underground coal mines. It also has a practical background with several extensive applications.

- **Keywords:** Dust distribution; Coal roadway; Air curtain; Euler-lagrange method; Numerical simulation

Sepideh Hosseinzadeh, Jan Berghmans, Jan Degreve, Filip Verplaetsen. *A model for the minimum ignition energy of dust clouds*. Pages 43-49.

This study refers to the minimum ignition energy (MIE) of dusts as determined by means of the Hartmann tube. To do so, six different dust with different particle size and properties are employed. A theoretical model is developed to predict the MIE based upon the physical and chemical properties of the dust. The model clearly shows the relationship between the minimum ignition energy and the minimum ignition temperature of a dust cloud. The model results in a method to calculate the MIE of dusts. Also, the time necessary for ignition can be calculated with the model. The results show that despite some limitations, the model predicts the MIE for dusts rather well. It is proposed that 40–60% energy loss would be considered when applying the model.

- **Keywords:** Minimum ignition energy; Dust clouds; Minimum ignition temperature; Theoretical model

Waqas Nawaz, Tomasz Olewski, Luc Véchot. *Assessment and validation of evaporation models for cryogenic liquids*. Pages 50-61.

The unanticipated release of cryogenic liquid is a serious safety risk since the vaporization of the cryogenic fuels may result in flammable vapor cloud which can lead to an explosion and/or fire. A significant amount of work has been carried out in the past to study the boiling phenomenon of cryogenic liquids. However, the evaporation of cryogenic liquid has not been thoroughly investigated. In reality, both of these phenomena are computationally equally important since during source term modeling, these two modes of vaporization are usually interchangeable. Incorrect source term prediction in any of these two regimes will result in poor estimation of consequences and hence will undermine the safety protocols. The interest to study evaporation mode of vaporization for cryogenic liquid stems from the fact that the boiling point of cryogens is below −150 °C and evaporation of cryogens will further decrease the temperature of the liquid, as observed through various evaporation models. However, these evaporation models have not been validated against the cryogenic liquid data. In order to fill this gap, the present study has three primary goals in context of cryogenic liquids: (i) understand and compare the existing evaporation models; (ii) evaluate the possibility of shift between boiling and evaporation regime; and (iii) validate the existing evaporation models. Six evaporation models were selected for this study through a comprehensive literature review. The behavior of the selected evaporation models was studied through a comprehensive parameter sensitivity analysis, including pool temperature, wind speed, ambient temperature, and pool size. Also, a medium scale experiment was performed, involving the spill of liquid nitrogen over polystyrene substrate, to observe the possibility of shift in the vaporization regime, and to validate the selected evaporation models. Although the results of the sensitivity analysis reflect on the possibility of evaporation of cryogenic liquids for some models, the experimental results confirm a complete absence of evaporation regime. Hence, based on the experimental results and sensitivity analysis, it was questioned through this work that the use of evaporation models in source term modeling may not be suitable for cryogenic liquids. However, more experiments should be carried out in future, on a larger scale, before coming to a general conclusion.

- **Keywords:** Cryogenic liquid; Source term modeling; Evaporation; Liquid nitrogen; Vaporization

Tae-In Ohm, Jong Seong Chae, Meng Yu Zhang, Seung Hyun Moon. *Effect of burner types and steam injection methods on thermal destruction of waste refrigerants (HFC-134a)*. Pages 62-68.

To minimize the high auxiliary energy consumption incurred in the thermal destruction process of waste HFC-134a, fuel, oxidants, refrigerants, and steam were injected into an incinerator in different forms, resulting in the development of an optimum burner. The new designed burner with two types of steam supply methods was used for comparing waste HFC-134a destruction characteristics. Two types of burners with 100% waste HFC-134a destruction efficiency during LPG (1.0 kg/h) combustion at excess air ratio of 1.1, were employed as auxiliary fuels. The results show: 1) internal temperature of the incinerator increases regardless of burner type when steam and waste HFC-134a are supplied at the same time, 2) maximum supply of waste HFC-134a is 2.8 kg/h in a destructor without steam supply, and 3) for injection of optimum steam supply (0.5 kg/h), the maximum rates of total thermal destruction of waste HFC-134a are 3.0 kg/h and 3.4 kg/h for type-1 and type-2 burners, respectively.

- **Keywords:** Waste HFC-134a; Incinerator; Refrigerant; Steam injection; Decomposition; Burner

Chaohang Xu, Deming Wang, Hetang Wang, Liyang Ma, Xiaolong Zhu, Yunfei Zhu, Yi Zhang, Fangming Liu. *Experimental investigation of coal dust wetting ability of anionic surfactants with different structures*. Pages 69-76.

To better understand the coal dust wetting ability of anionic surfactants with different structures, sodium dodecyl sulfate (SDS), sodium dodecyl sulfonate (SDDS), and sodium dodecyl benzene sulfonate (SDBS) were selected. The surface tension, wetting time, and infrared spectra of coal dust were tested. The hydrophilic-lipophilic balance (HLB) values of the surfactants were calculated. Results showed that the decrease in the surface tension could shorten the wetting time at low surfactant concentrations. But the decrease in the wetting time was no longer related to the constant surface tension that was lower than 45 mN/m. The adsorption density depends on the hydrophobic interactions and electrostatic repulsions between the surfactant molecules and the coal dust. During the dynamic immersion process, the surfactants with high HLB values could bring the coal dust into the bulk solution rapidly. The wetting time of coal dust for SDBS with a high adsorption density and low HLB or SDS with a small adsorption density and high HLB was relatively longer. The adsorption density and HLB value of SDDS were intermediate between those of SDS and SDBS. Under the combined action of these two factors, the wetting time of SDDS was shorter than those of SDS and SDBS.

- **Keywords:** Coal dust; Anionic surfactant; Wetting time; Surface tension; Adsorption density; Hydrophilic-lipophilic balance

Abbas Hemmati, Hamed Rashidi. *Optimization of industrial intercooled post-combustion CO2 absorber by applying rate- base model and response surface methodology (RSM)*. Pages 77-86.

The most important challenge in the post-combustion CO2 capture process is energy consumption. Using intercooled absorption columns increases absorption rate and decreases the energy needed for solvent regeneration. In this study, the optimum conditions for the usage of intercoolers (height and duty) have been investigated. First of all, the accuracy of rate-base model was validated to predict industrial unit in four different situations. The results showed that CO2 absorption percentage and temperature along the height of the absorption column were predicted precisely with average error of 1.38% and 3.85%, respectively. The second part of this article is dedicated to the optimization to maximize CO2 absorption and minimize total cooling duty by applying response surface methodology (RSM). The statistical analysis showed that the optimum heights for intercoolers I and II were found to be 2 and 5 m, respectively. The energy consumption of intercoolers I and II in optimum conditions were -496 and -809.28 kW

respectively. By applying intercoolers' optimum conditions in the model, the CO2 absorption percentage and energy consumption were obtained at 87.29 and −3890 kW, respectively. Hence, by decreasing the intercoolers' height in the absorption column and using intercoolers in the optimum heat duty, with constant packing height, the CO2 absorption increased by 3.3%.

- **Keywords:** Post-combustion CO2 capture; Rate-base model; Intercooled absorber; Response surface methodology (RSM); Absorption percentage; Energy consumption

Pooya Arbab, Bita Ayati, Mohammad Reza Ansari. *Reducing the use of nanotitanium dioxide by switching from single photocatalysis to combined photocatalysis-cavitation in dye elimination*. Pages 87-93.

The present study was conducted to investigate the elimination of Reactive Black 5 (RB5) through the photocatalytic process alone and a combination of photocatalysis and cavitation using nanotitanium dioxide as a photocatalyst. To use a new form of cavitation, hydrodynamic cavitation (HC) was generated by an orifice plate with a 7 mm hole diameter at the inlet pressure of 4 bars. First, the photocatalytic process was optimized by changing the parameters of pH, nanotitanium dioxide concentration, irradiation power and dye concentration; then, by adding cavitation and producing combined photocatalysis-cavitation and with the same optimal conditions obtained in the previous stage, the amount of nanophotocatalyst was adjusted, and the amount of nanotitanium dioxide required to yield an efficiency equal to that of the single process was calculated. Finally, by measuring the amount of current consumed in these processes, the cost of nanotitanium dioxide and the electrical energy consumption, the total cost of both the single and the combined processes was estimated in the same efficiency. The results showed that using cavitation significantly reduces the amount of nanomaterials used from 100 to 8.4 mg/L and the total cost of the process to one-seventh, which suggests that cavitation is a very promising process.

- **Keywords:** Reactive Black 5; Photocatalytic process; Hydrodynamic cavitation; Nanotitanium dioxide; Orifice plate; Cost

Abhishek Sharma, Yashvir Singh, Gyanendra Kumar Singh, Abrham Talargie Habte, Nishant Singh. *Production of polanga methyl esters and optimization of diesel engine parameters through response surface methodology approach*. Pages 94-102.

More demand for fossil fuel and significant increase in the air pollution levels due to combustion of the fossil fuel provides an opportunity to discover some clean and environmental friendly fuels for the engines. The present work is focused on the optimization of engine operating parameters to result in the optimum increase in the efficiency of the engine running on polanga biodiesel blends. The fuel injection pressure, fuel injection timing, polanga based biodiesel blends, and engine load were considered as input parameters for the optimization of brake thermal efficiency (BTE), unburnt hydrocarbon (UHC), and NOx emission. Experiments were conducted as per the central composite rotating design (CCRD) matrix. The optimum combination of input parameters for maximum brake thermal efficiency and minimum exhaust emissions were found at fuel injection timing 15°bTDC, fuel injection pressure 196.36 bar, 40% biodiesel blend (B40) and 53% engine load. Experimental and optimized results at the prescribed optimum setting were compared and the error percentage were found within the limit of 5%.

- **Keywords:** Polanga biodiesel; Response surface methodology; Engine performance

Gona Hasani, Afshin Maleki, Hiua Daraei, Reza Ghanbari, Mahdi Safari, Gordon McKay, Kaan Yetilmezsoy, Fatih Ilhan, Nader Marzban. *A comparative optimization and performance analysis of four different electrocoagulation-flotation processes for humic acid removal from aqueous solutions*. Pages 103-117.

Humic substances (HSs) are a group of complex macromolecular polymeric compounds originating from the decomposition of plant residuals and other organic matter. Within the presence of micro-pollutants and heavy metals, HSs negatively act upon potable water quality by contributing to aesthetic problems such as yellowish or brownish color and annoying taste and odor. They are also responsible for re-growth of pathogenic microorganisms and fouling of membranes in water distribution systems. More importantly, these high-molecular-weight polymers have been noted to be the major contributor to the formation of disinfection by-products (DBPs) such as trihalomethanes (THMs) and haloacetic acids (HAAs). Considering these harmful effects, removal of HSs is one of the significant tasks in drinking water treatment. For this purpose, this study aimed to explore the effects of various operating parameters (initial concentration, initial pH, electrical conductivity, pulse time, pulse number, and process time) on the humic acid (HA) removal efficiency and energy consumption. In this study, a new current supply method called alternating pulse current electrocoagulation-flotation (APC-ECF) process was proposed, and a detailed comparative optimization of four different ECF processes (direct current (DC)-simple electrode, DC-perforated electrode, pulse current-simple electrode, and pulse current-perforated electrode) was conducted within the framework of Taguchi-based experimental design methodology. According to scanning electron microscopy (SEM), the morphology of electrode surfaces with APC and perforated electrode showed less disordered (irregular) pores and a regular structure of aluminum compared to the DC, which confirmed the difference in the corrosion rates. Moreover, the proposed APC-ECF method led to the production of less dewatered and dense sludge. The results of the performance analysis revealed that the APC with a perforated electrode provided 3.2-fold lower energy consumption and 2.5-fold lower aluminum consumption compared to the DC with a simple electrode. Considering the expenses associated with power consumption and sludge disposal costs for the electrocoagulation unit, the experimental findings corroborated that the proposed APC-ECF process could be used as a promising and cost-effective technology in water treatment for the removal of HSs.

- **Keywords:** Alternating pulse current; Electrocoagulation-flotation; Electrode morphology; Humic acid; Design of experiments; Taguchi method

Hongbin Qiu, Mengliang Wang, Yingming Xie, Jianfeng Song, Tao Huang, Xue-Mei Li, Tao He. *From trace to pure: Recovery of scandium from the waste acid of titanium pigment production by solvent extraction*. Pages 118-124.

The waste acid from the titanium pigment production process contains scandium ion at low concentration. The waste is thus an extra resource for scandium. To recover the trace scandium from the waste acid, a process combining pre-enrichment and purification steps via solvent extraction using the extractant of bis-(2-ethylhexyl) phosphoric acid was reported. In the pre-enrichment step, to obtain high extraction efficiency at low extractant consumption, the volume fraction of bis-(2-ethylhexyl) phosphoric (as extractant), tributyl phosphate (as synergistic agent) and the ratio of aqueous-to-organic extractant (A/O) were optimized. Afterwards, to remove the main impurities from the enriched liquor, the further purification step was investigated. Herein, to improve the separation between scandium and titanium, (TiO)2+ was transformed to [TiO(H2O2)]2+ by addition of H2O2 into the pre-enriched liquor prior to extraction. The co-extracted metal ions were subsequently scrubbed with 3 mol/L H2SO4/6% H2O2 by multi-stage

cross-current. Further, the extractant was reused for four cycles and the extraction efficiency for scandium was found to be stable after the third cycle. Based on current results, a process to recover the trace scandium from real titanium white waste acid was introduced on lab scale as a proof of principle.

- **Keywords:** Scandium; Titanium white waste acid; Solvent extraction; D2EHPA; [TiO(H2O2)]2+

Gelavizh Barzegar, Junxue Wu, Farshid Ghanbari. *Enhanced treatment of greywater using electrocoagulation/ozonation: Investigation of process parameters*. Pages 125-132.

In current work, electrocoagulation (EC)/ozone process was applied for the treatment of greywater. The effects of several parameters were studied on chemical oxygen demand (COD) and total organic carbon (TOC) removals from greywater. The results showed that 85% of COD and 70% of TOC were removed during 60 min electrolysis time, at pH = 7.0, 47.4 mg/L ozone and 15 mA/cm2 current density. EC with Fe electrode exhibited high catalytic activity for ozone activation in contrast with Al electrode. According to the results, ozone had a superior compared to other chemical oxidant (peroxidisulfate, peroxymonosulfate and hydrogen peroxide) in combination with EC process for greywater treatment. UV irradiation improved the performance of EC/ozone considerably while ultrasound could not affect EC/ozone process. In the presence of UV irradiation, 95% of COD and 87% of TOC were eliminated. Moreover, 4 logs of total coliform and 96% of Escherichia coli were removed by EC/ozone/UV process. The calculated costs of EC/ozone and EC/ozone/UV were 1.9 and 4.03 $/m3 respectively. Hereupon, current system is an efficient and executable process for the treatment and disinfection of greywater.

- **Keywords:** Greywater; Electrocoagulation; Disinfection; UV irradiation; Ozonation

Chigozie Francolins Uzoh, Okechukwu Domnic Onukwuli, Ikenna Henry Ozofor, Raphael Stone Odera. *Encapsulation of urea with alkyd resin-starch membranes for controlled N2 release: Synthesis, characterization, morphology and optimum N2 release*. Pages 133-142.

Nitrogen released into soils from uncoated urea granules is lost continuously due to volatilization, leaching, denitrification, nitrous emission, water eutrophication and surface run-off. Reducing the release rate can increase its efficiency of use and reduce nitrogen pollution. In this research, granular urea fertilizer was encapsulated with alkyd resin-starch bio-composites as materials of biodegradable and regenerative resources to obtain controlled release coated urea (CRCU). Different bio-composites were synthesized from each of castor seed oil and rubber seed oil based alkyd resin (modified with sorbitol, maleic and phthalic anhydride) and cassava starch. Effects of sorbitol, maleic anhydride and pthalic anhydride on the release kinetics of the CRCU were evaluated. Optimum nitrogen release characteristic of the CRCU was evaluated as a function of coating thickness, release time and pH. Structural and morphology elucidation of the raw urea and encapsulated ureas were established using FTIR and SEM instrumental analysis, respectively. Nutrient release kinetic of the different coated urea was determined using Kjeldahl method. FTIR result confirmed the esterification reaction and hydrogen bonding integrity of the alkyd resins and starch. The SEM images of the raw urea appears rough and have fine openings while that of CRCUs possess a seemingly decrease in membrane porosity and ordered uniform layer. 31.66 and 48.61% cumulative nitrogen release were obtained with coating thickness of 6.4(mm), time of 24 days, pH of 8 and 2.2(mm), time of 24 days, pH of 8 for RSO-St-S and CSO-St-S encapsulated urea, respectively. The encapsulated ureas perfectly satisfy the requirements of European Standard EN 13,266 for CRFs. It can be concluded that the synthesized CRCU efficiently retard nitrogen release.

- **Keywords:** Controlled release; Encapsulation; Response surface methodology; Biodegradable; Release kinetics; Process optimization

Abhilash T. Nair, Jaganathan Senthilnathan, S.M. Shiva Nagendra. *Emerging perspectives on VOC emissions from landfill sites: Impact on tropospheric chemistry and local air quality*. Pages 143-154.

Adverse impacts of volatile organic compounds (VOCs) released from the landfill sites into the atmosphere is a major concern in most urban areas. There exist a limited information on the effects of VOCs emitted from open dumpsite particularly for tropical climatic conditions. The present study reviews the source, concentrations and pathways of VOCs released from landfill sites into air and summarises their impacts on surrounding environment and nearby residents. Further, it provides insight on generation of secondary pollutants due to photochemical reactions between the VOCs released from landfill sites and compounds already existing in troposphere. VOCs released from landfill sites can undergo photochemical reactions with the hydroxyl radicals and NOx present in the troposphere to form O3, secondary organic aerosols (SOA) and intermediate products, which can deteriorate the air quality. Nevertheless, studies using mathematical simulation augmented by suitable laboratory experiments and continuous monitoring data can aid in detailed analysis on the mechanism of the secondary pollutant formation by VOCs emitted from the landfill sites. Findings of this study will open new avenue of research for further investigations on pathways of photochemical reactions of VOCs released from the landfill sites leading to secondary pollutant formation in proximate surface environment.

- **Keywords:** Municipal solid waste; Landfilling; Volatile organic compounds; Ozone formation; Secondary pollution

Zhihong Yin, Yunguo Liu, Xiaofei Tan, Luhua Jiang, Guangming Zeng, Shaobo Liu, Sirong Tian, Sijia Liu, Ni Liu, Meifang Li. *Adsorption of 17β-estradiol by a novel attapulgite/biochar nanocomposite : Characteristics and influencing factors*. Pages 155-164.

A novel attapulgite/biochar (ATP/BC) nanocomposite was synthesized via simultaneous activation and carbonization for 17β-estradiol (E2) removal in water. The one-step synthetic process significantly enlarged specific surface area and increased oxygen-contained functional groups. Compared to the pristine biochar (BC) and attapulgite (ATP), the ATP/BC nanocomposite exhibited higher adsorption capacity for E2 with the maximum adsorption capacity (qmax) of 154.23 mg/g. The pseudo-second-order and Langmuir model were more suitable for E2 adsorption by ATP/BC. The adsorption capacity of ATP/BC for E2 was affected by initial solution pH and the low pH was favorable for the adsorption of E2. The presence of monovalent cations (Na+ and K+) improved the adsorption efficiency for E2, whereas the presence of divalent cations of (Ca2+ and Mg2+) inhibited the adsorption process of E2. Ionic strength had slight promoting effect at low concentration for the E2 adsorption. The presence of surfactant and humic acid inhibited the adsorption capacity of ATP/BC. Electrostatic attraction, π-π interactions and hydrogen bonds between ATP/BC and E2 molecules might be potential adsorption mechanisms. The results showed that the ATP/BC nanocomposite was a high efficiency and reusable adsorbent in the removal of E2 from water.

- **Keywords:** Attapulgite; Biochar; Adsorption; 17β-estradiol; Characteristics

Tawfik A. Saleh, Saddam A. AL-Hammadi, Adnan M. Al-Amer. *Effect of boron on the efficiency of MoCo catalysts supported on alumina for the hydrodesulfurization of liquid fuels*. Pages 165-174.

The effect of boron content on hydrodesulphurization (HDS) activity was investigated under different optimized conditions. γ-Al2O3 was loaded with MoCo and then doped with boron. The obtained materials, i.e. AlMoCoB0%, AlMoCoB2%, and AlMoCoB5% were characterized by N2-physisorption, X-ray diffraction, temperature programmed analysis by reduction and desorption, Fourier-transform infrared spectroscopy, a scanning electron microscopy, transmission electron microscopy, and thermogravimetric analysis. The catalytic activity of the prepared catalysts was evaluated for the HDS of dibenzothiophene (DBT) using a Parr batch reactor at T = 300 °C and under 50 bar hydrogen partial pressure. The textural properties of the prepared catalysts were enhanced by introducing the boron. For example, the BET surface area of AlMoCoB5% was 206 m2/g which is higher than that of both AlMoCoB0% and AlMoCoB2%. The acidity and dispersion AlMoCoB5% were 0.77 and 2.46 (mmol/g), respectively, which increase its HDS activity. The boron enhanced the particle dispersion, leading to an improvement in the catalytic activity of the MoCo catalysts in the elimination of sulfur content. Experimental factors (such as temperature, pressure, the dosage of the catalysts and contact time) were investigated and optimized using a central composite design. The results revealed that the HDS was improved by increasing the temperature, pressure, and catalyst dosage. The optimum contact time was found to be 6 h with a dosage of 0.6 g. The experimental results indicated that AlMoCoB5% has the highest HDS activity, achieving more than 98% of sulfur removal, which is below the allowed sulfur level. The excellent catalytic activity of the AlMoCoB5% catalyst in the HDS of DBT is particularly useful for the ultradeep HDS of fuels.

- **Keywords:** Oil; Deep hydrodesulfurization; Boron; Acidity; Catalyst; Thiophene

Tao Lu, Ying Chen, Min Liu, Wenju Jiang. *Efficient degradation of evaporative condensing liquid of shale gas wastewater using O3/UV process*. Pages 175-183.

In this study, a batch experiment was used to investigate the degradation of real evaporative condensing liquid of shale gas wastewater (ECLSGW). We showed that compared to the O3, ultraviolet (UV), UV/TiO2, and O3/UV/TiO2 processes, the O3/UV process has better performance in removing the chemical oxygen demand (COD) and total organic carbon (TOC) of ECLSGW under the same conditions. The effects of initial pH (3–12), ozone flow rate (0.1–0.5 L/min), UV power (15–50 W), and reaction time (0–60 min) on the degradation of ECLSGW via the O3/UV process were investigated using a single-factor experiment. Moreover, the optimal experimental conditions were obtained using a quadratic polynomial prediction model (RAdj2=0.9961) that was obtained from the central composite design (CCD) of the response surface methodology (RSM). Under optimal experimental conditions, the COD and TOC removal efficiency reached 93.12 and 95.5%, respectively. In addition, gas chromatography–mass spectrometry analysis showed that the O3/UV process could nearly completely mineralize organic pollutants in the ECLSGW. Hydrogen peroxide (H2O2) and hydroxyl radical (OH) were identified by manganese dioxide (MnO2) and tert-butanol (TBA). The mechanism research showed that OH plays an important role in the degradation of organic pollutants. In summary, the O3/UV process is an effective method to degrade ECLSGW.

- **Keywords:** Shale gas wastewater; O3/UV; Response surface methodology; Synergistic effect; Reaction mechanism

Mohammad Amin Boojari, Seyed Morteza Zamir, Seyed Abbas Shojaosadati. *Transient-state strategies for the removal of toluene vapor in a two-liquid phase biotrickling filter: Experimental study and neural network analysis*. Pages 184-193.

The performance of a two-liquid phase biotrickling filter (TLP-BTF) packed with pall ring and pumice in the presence of silicone oil, as the organic solvent (10% v/v), was evaluated for the treatment of toluene vapor under various transient conditions. The experiments were done at EBRT of 1 min and inlet loading rates (ILRs) of 150-180 g m^{-3} h^{-1} and comprise of shock loading, intermittent loading for 10 h day-1, and aeration without toluene loading during shutdown periods. The TLP-BTF removal efficiency (RE) attained steady state (RE = 66%) in less than 40 min after loading initiation in different operating strategies. The TLP-BTF was subjected to a 5.5-fold increase at ILRs from 34 to 186 g m^{-3} h^{-1}, however, RE declined only 10% within 2 h after shock loading. Nevertheless, RE decreased to 44% due to dominating the kinetic-limitation regime and silicone oil saturation. The variations of TLP-BTF performance were analyzed by using artificial neural networks (ANNs) modeling by means of casual index (CI) values. Lower discrepancies for CI-values in TLP-BTF (-8.05 > CI > -10.68) in comparison to the single-liquid phase BTF (-9.19 > CI >14.04) indicated the role of silicone oil for decreasing the negative impact of different intermittent loading types on the BTF performance.

- **Keywords:** Sensitivity analysis, Silicone oil, Mass transfer, Intermittent loading, Casual index

Tsz Him Kwan, Khai Lun Ong, Md Ariful Haque, Sandeep Kulkarni, Carol Sze Ki Lin. *Biorefinery of food and beverage waste valorisation for sugar syrups production: Techno-economic assessment*. Pages 194-208.

Techno-economic analysis was conducted to evaluate a food and beverage (F&B) waste valorisation process for sugar syrup production via integrated biorefinery. A comprehensive process model was developed with a capacity of 10 metric tons (MT) $hour^{-1}$ of food waste and 14 MT $hour^{-1}$ of beverage waste. Three scenarios were proposed with different types of sugar syrups as the main products: Scenario I) fructose syrup, Scenario II) high fructose syrup-42, and Scenario III) glucose-rich syrup. Mass balance showed conversion yields of 0.24 MT sugar syrups per MT of F&B waste, while lipids (0.07 MT per MT of F&B waste) and insect feed (0.44 MT per MT of F&B waste) were the co-products proposed to be used for other industrial biorefinery processes. All scenarios were observed to be economically self-sustainable with net profit generation (US$11-26 million $year^{-1}$) and positive net present values (US$92-294 million). Along with the net production costs (US$443-665 MT^{-1}), the sugar syrups derived from the F&B waste have relatively low minimum selling prices of US$157-747 MT^{-1} at a 5% discount rate. Lastly, sensitivity analysis was performed which found that the prices of sugar syrups were the largest determinants of their profitability. This study proposes a significant techno-economic basis for F&B waste biorefinery, which offers a successful demonstration for food and drink industries adopting these biotechnological processes for the same plant size.

- **Keywords:** Food and beverage waste; Fructose; Glucose; Purification; Saccharification; Sensitivity analysis

M.A. Martín-Lara, A. Pérez, M.A. Vico-Pérez, M. Calero, G. Blázquez. *The role of temperature on slow pyrolysis of olive cake for the production of solid fuels and adsorbents*. Pages 209-220

In this work, slow pyrolysis of olive cake has been carried out under nitrogen atmosphere at different temperatures to obtain carbonaceous materials with possible applications as solid fuels and adsorbents of heavy metals from aqueous solutions. The carbonaceous materials have been completely characterized. The Gain and Loss method has been applied in order to find the best operating temperature in terms of quality of the carbonaceous material for its use as fuel. Also, a basic reaction scheme has been proposed for representing the kinetics of thermal degradation in nitrogen and air atmospheres. Good correlation of calculated and experimental data was observed for

different materials. Finally, adsorption experiments were performed to test ability of carbonaceous materials as adsorbents of cadmium, chromium, copper, nickel and lead. In general, the carbonaceous solids obtained by slow pyrolysis improved the adsorption capacities of the raw material. For example, a maximum lead adsorption capacity of 102 mg/g was found for carbonaceous material obtained at 450 °C. Also, for this material, the values of maximum adsorption capacity indicated the higher preference of solid for lead ions.

- **Keywords:** Olive cake; Slow pyrolysis; Solid fuels; Adsorbents; Heavy metal removal

Hamed Taghvaei, Mohammad Reza Rahimpour. *Catalytic hydrodeoxygenation of bio-oil using in situ generated hydrogen in plasma reactor: Effects of allumina supported catalysts and plasma parameters*. Pages 221-228.

In this study, hydrodeoxygenation of guaiacol, a lignin derived model compound, has been studied experimentally via a combination of dielectric barrier discharge plasma and catalyst. Cracking of methyl groups in the chemical structure of bio-oil is used to provide the hydrogen which is required for hydrodeoxygenation reaction. In order to maximize the degree of deoxygenation and guaiacol conversion, the effects of operating and plasma parameters including applied voltage, guaiacol and argon flow rate have been examined. Furthermore, performance of plasma alone and catalytic plasma has been compared by filling the active volume of the discharge with different commercial catalysts including Ni, Co–Mo, Ni–Mo, Pt–Re and Pt–Cl supported on Al2O3. The highest guaiacol conversion of 92% and deoxygenation degree of 65% are achieved in the presence of Pt–Cl/Al2O3 and Pt–Re/Al2O3 catalysts, respectively. According to the results, the main products were BTX, phenol, methylphenols and dimethylphenols. Unlike previous studies in which catechol was produced as a major product, in our plasma system phenol can be produced selectively through direct demethoxylation rather than demethylation reaction. It is also evident from the results that the hydrogen challenges of hydrodeoxygenation reaction can be overcome by catalytic DBD plasma reactor.

- **Keywords:** Biomass; Bio-oil; In situ hydrogen production; Upgrading; Non-thermal plasma; Catalyst

Mayur Shirish Jain, Siddhartha Paul, Ajay S. Kalamdhad. *Utilization of Biochar as an amendment during lignocellulose waste composting: Impact on composting physics and Realization (probability) amongst physical properties*. Pages 229-238.

The lower moisture content and bulk densities characterize the Biochar. It is rich in carbon and possesses higher porosity. Utilization of Biochar during composting of various organic wastes successfully improved the efficacy of the composting process, degradation rate, and final product quality. However, the composting physics during the composting of lignocellulose aquatic waste is rarely studied. Hence the objective of this research is to assess the impact of biochar addition (0 and 2.5% w/w) to a mixture of Eicchornia Crassipes, cow dung, and sawdust. The study provides an insight of composting physics, percentage improvement rate of degradation of organic matter, and the cation-exchange capacity. As a result of Biochar addition, the thermophilic (57.3 °C) temperature lasted for more than three days. The Biochar addition decreased the bulk density by 7% in the initial feedstock. It also aided in increasing the initial value of the free air space and porosity of the mixture. The study noted a strong relationship amongst physical parameters and the significant correlation of degradation of organic matter with moisture content and bulk density ($p < 0.05$). This study would provide valuable information for improving physical properties during application of compost to the soil.

- **Keywords:** Composting; Eichhornia Crassipes; Biochar; Moisture content; Bulk density; Probability

Nafiz Tamim, Delphine M. Laboureur, A. Rashid Hasan, M. Sam Mannan. *Developing leading indicators-based decision support algorithms and probabilistic models using Bayesian network to predict kicks while drilling*. Pages 239-246.

Predicting a kick timely and efficiently is often a challenging task due to the complexities of drilling and other well intervention activities. This work proposes a leading indicators-based approach to assess drilling operations for predicting kicks and preventing blowouts. A cause-based methodology is proposed to develop sets of leading indicators for different categories and organizational levels. Leading indicators are divided into two broad sections – real-time indicators and long-term organizational safety performance indicators. With the real-time indicators, various decision support algorithms are developed which would help to understand a kick progression scenario effectively. Probabilistic barrier failure models for different stages of drilling are also developed to assess performance of primary well control barrier – hydrostatic head. To predict barrier failure events effectively, Bayesian network models are developed combining organizational, operational and real-time indicators. The probability distribution for observing changes in real-time parameters when a kick is in progression are also determined. This study would allow both predictive (causes to effects) and diagnostic (effects to causes) reasoning of kicks and blowouts for better understanding of well control system while drilling. Developed risk models enable informed decision making with a relatively clear picture of the risk of barrier failure and provide useful information on actions required to prevent escalation of well control events.

- **Keywords:** Leading indicators; Decision support algorithms; Probabilistic models; Bayesian network; Drilling kicks

Qiujian Lin, Da Kang, Meng Zhang, Tao Yu, Dongdong Xu, Zhuo Zeng, Ping Zheng. *The performance of anammox reactor during start-up: Enzymes tell the story*. Pages 247-253.

Start-up is the first and essential step in the operation of anammox (anaerobic ammonia oxidation) reactor. It is helpful to know the progress of start-up for the real-time optimization of reactor performance. In this work, a start-up mode was successfully established, by which the anammox reactor was smoothly put into use, with NLR (Nitrogen Loading Rate) and NRR (Nitrogen Removal Rate) of 11.0 and 10.1 kg-N /(m3 d), respectively. During the start-up, the dehydrogenase, alkaline phosphatase, hydrazine oxidase and heme of the anammox granular sludge were investigated and their activity/content was correlated with the reactor performance. The activity of dehydrogenase and alkaline phosphatase was found to decrease with the elevation of NLR. On the contrary, the hydrazine oxidase activity and heme content were observed to increase with the elevation of NLR. Based on the relative enzyme level, an enzyme indicator system was created to monitor the start-up progress of anammox reactor.

- **Keywords:** Anammox; Start-up; Dehydrogenase; Alkaline phosphatase; Hydrazine oxidase; Heme

Salawu Omobayo Adio, Mohammad Asif, Abdul-Rashid I. Mohammed, Nadeem Baig, Abdulrahman A. Al-Arfaj, Tawfik A. Saleh. *Poly (amidoxime) modified magnetic activated carbon for chromium and thallium adsorption: Statistical analysis and regeneration*. Pages 254-262.

The study discusses the use of magnetic activated carbon modified with poly (amidoxime) (PAMC) as an efficient approach for the adsorption of chromium and thallium. Activated carbon was synthesized from waste rubber tires, subsequently enhanced with magnetic properties, and modified with poly (amidoxime) providing more functional groups and thus improve the sorption efficiency. The morphological and structural properties of the prepared materials were investigated using different characterization techniques including SEM-EDX, BET, and FTIR. The adsorption evaluation was carried out in accordance with a factorial design to determine the optimum condition for the removal process. Factorial design analysis ensures the use of limited resources while also obtaining the optimum efficiency of the adsorption process. A half factorial design method was adopted in this study. The conditions varied include; pH, the initial concentration of adsorbent, shaker speed, contact time and adsorbent dosage. The material showed high efficacy within a wide pH range (3–11) even with a small dosage of 1 g/L. Interestingly, the material showed good efficiency for the uptake of the test toxic metal ions at low and high concentrations of 1 and 20 ppm with acceptable statistical values. Shaker speed of 200 rpm was the optimum. More than 97% of the chromium was removed using each of 1 and 5 g/L of the adsorbent. Analysis of variance showed a high correlation for the removal process with p-values < 0.003 for the removal of thallium. To demonstrate how the material can be used in process engineering design and practice, regeneration of PAMC and the fate of the adsorbates were evaluated. Tests were also conducted using real wastewater. With easy separation and high efficiency of removal for both chromium and thallium from water and good regeneration without showing a significant loss in adsorption capacity even after several cycles, the material demonstrated its exciting potential as an adsorbent for water treatment.

- **Keywords:** Clean technology; Environmental management; Water treatment; Statistical analysis

Lu-Qing Wang, Hong-Hao Ma, Yong-Xing Deng, Zhao-Wu Shen. *On the detonation behavior of methane-oxygen in a round tube filled with orifice plates*. Pages 263-270.

In this study, the detonation behaviors of stoichiometric methane-oxygen mixture were examined in a round tube filled with orifice plates. The blockage ratio was 0.56 and the plate spacings were 1, 1.5 and 2 times the tube diameter. Detonation velocity measurement and soot foils were adopted to study the propagation characteristics. Experimental results show that the abrupt velocity jump was only observed for the obstacle configuration with S=2D, where S and D are the plate spacing and the tube diameter. For a fixed plate spacing, the detonation velocity as well as the detonation limits are independent of the orifice geometry, since the effective diameters (deff) of the orifices are almost the same. The ratios of deff to the detonation cell size (λ) were found to be 0.4–0.5. For sensitive mixtures, the soot foils indicate that the detonation re-initiation occurs via hot spots formed on the wall. As the initial pressure decreases, the detonation can travel without hot spots generation. At the limits, no indication of detonation can be observed for obstacle configurations with smaller spacings in spite of the higher velocity (compared with the isobaric sound speed of the products). The propagation mechanism near the limits is left, however, for further investigation.

- **Keywords:** Methane-oxygen; Detonation propagation limits; Orifice plates; Cellular structure

Syaza I. Ahmad, Haslenda Hashim, Mimi H. Hassim, Roslina Rashid. *Development of hazard prevention strategies for inherent safety assessment during early stage of process design*. Pages 271-280.

A safety program that prevents hazards from occurring is preferable than the typical approaches of eliminating hazards upon being detected. Chemical plants should be

designed so that they are user-friendly and exhibit good safety features to prevent accidents. This can be done by preventing the presence of hazards in the process fundamentally, which is formally known as the inherent safety concept. This paper discusses the development of process hazard prevention strategies (HPS) during the early design stage. The strategies were formulated into a detailed framework which was constructed using thematic analysis. The thematic analysis was used to extract hazard prevention strategies from the accident databases – producing results in the form of keywords, referred here as themes and generated codes. Common keywords that appeared in the accident databases on how to prevent the accidents were gathered and referred to as generated codes in this research. The generated codes were then grouped into five themes namely; materials, design, operating, chemicals and control. This study was applied to the case study of benzene production from toluene involving separation and heat transfer equipment. The HPS themes identified for separation equipment were design, operating and chemicals, while for heat transfer equipment the themes identified were materials, design, operating, chemicals and control. This technique produced similar results as two other techniques on the Bhopal case study and the toluene nitration case study, with justified differences. This not only proves the effectiveness of the framework but also supports the validity of the framework.

- **Keywords:** Inherent safety; Hazard prevention; Thematic analysis; Accident databases; Early design stage

Malin Song, Shuhong Wang, Liang Lei, Li Zhou. *Environmental efficiency and policy change in China: A new meta-frontier non-radial angle efficiency evaluation approach*. Pages 281-289.

This study revised the non-radial angle model and set up the meta-frontier non-radial angle efficiency (MNAE) model. Moreover, an angle efficiency index was established in the MNAE model to reflect changes in the production decisions of decision-making units as a result of the external environment. The study conducted empirical analysis on data for 30 provinces in China from 2004 to 2015. The results showed that the eastern area of China was sensitive to fluctuations in the world's economy and was able to quickly adjust production decision making; the western area lagged relatively behind in making changes, and the central area was not affected. Effects of international trade and foreign direct investment on the Shandong, Jiangsu, Fujian, Liaoning, Hunan, Henan, Jiangxi, and Sichuan provinces were significant and caused notable policy changes, which led to short-term resource waste and policy faults. This study also provides policy advice based on the results.

- **Keywords:** Non-radial; Angle efficiency; DEA; Environmental efficiency; Meta-frontier

Syed Ali Mehdi Naqvi, Muhammad Raza, Vincent T. Ybarra, Saeed Salehi, Catalin Teodoriu. *Using content analysis through simulation-based training for offshore drilling operations: Implications for process safety*. Pages 290-298.

Human factors play a large role in the creation and optimization of process safety in offshore drilling and well control operations by assessing and mitigating human error. The current industry practice relies on the simulation-based trainings for its drilling crews which lack the measurement and evaluation of human factors and non-technical skills. One way to improve training is to measure and evaluate an individual's performance and non-technical skills, but there are no such validated, psychological tools made for offshore drilling operation. A way to create these tools is with the use of the content analysis and process tracing techniques, which are frequently used in research to identify psychological processes via communication. This paper presents the potential use of

content analysis as a tool to optimize simulation-based trainings that can be applied to improve human factors in drilling and well control activities. To put this to test, an interactive trip-in experiment was specially designed in the University of Oklahoma virtual reality drilling simulator that allowed four participants as assistant drillers (two Novices and two Experts) to individually engage in four similar simulations and communicate with a driller in a manner similar to a real-world setting. The results from content analysis were translated into semantic maps to explore individual psychological states which informs their cognitive processes (e.g. working memory, long-term memory, metacognition) used during the experiment. The research found significant differences in the problem-solving techniques for the Novices and the Experts meaning, that perhaps they approached the problem psychologically differently. Results are a proof of concept that content analysis is an additional tool that may allow for improved performance evaluation and human factors optimization through simulation-based trainings.

- **Keywords:** Simulation-based training; Process safety; Content analysis; Human factors; Offshore drilling

Mira Milinković, Blažo Lalević, Jelena Jovičić-Petrović, Vesna Golubović-Ćurguz, Igor Kljujev, Vera Raičević. *Biopotential of compost and compost products derived from horticultural waste—Effect on plant growth and plant pathogens' suppression*. Pages 299-306.

Besides ecological and environmental benefits of green open spaces, horticultural waste management has various environmental consequences. Green waste composting represents promising environmentally friendly alternative which gives valuable products with positive soil and plants impact. Composting products' quality determinates their application and depends on the particular waste material and process parameters. The aim of this paper was to estimate the chemical and microbiological quality of green waste compost and compost products (compost tea, compost extract and the solid phase after extraction), and their biopotential based on germination rate, germination index and inhibition of phytopathogenic fungi growth. Higher germination rate of examined plant seeds was noticed on the solid phase after extraction, and compost extract, compared to compost, and compost tea, respectively. Plants with low germination rate grown on compost showed higher fresh and dry biomass. Compost products strongly inhibited the growth of plant pathogens Fusarium oxysporum, Rhizoctonia sp., and Pythium debaryanum. Presented results show that composted biodegradable waste from urban green spaces contribute to the plant growth and phytopathogenic fungi suppression, and thus improve the overall environmental quality.

- **Keywords:** Green waste; Compost; Compost products; Phytopathogenic fungi suppression; Germination rate

Song Xin, Long Zhang, Xiaona Jin, Qi Zhang. *Reconstruction of the fault tree based on accident evolution*. Pages 307-311.

Fault tree analysis (FTA) is an important analysis method in safety system engineering, however, the method only can be used to analyse a specific accident but cannot analyse the whole generation and development process behind it. After the occurrence of top event, the consequence of the original accident probably expands to result in the expansion of the accident owing to the appearance of some specific factors. Aiming at this, the concept of an evolving fault tree is proposed to rationalise the original fault tree. By undertaking consequence reasoning, the evolving fault tree is constructed based on the original fault tree. Afterwards, through qualitative and quantitative computation of the evolving fault tree, the accident cause and logical relationship between accident factors are further revealed to identify control points for accidents. This helps when reducing, and even precluding, the occurrence of accidents.

- **Keywords:** Fault tree reconstruction; Evolving fault tree; Consequence reasoning; Qualitative analysis; Safety

Fereshteh Jaderi, Zelina Z. Ibrahim, Mohammad Reza Zahiri. *Criticality analysis of petrochemical assets using risk based maintenance and the fuzzy inference system*. Pages 312-325.

Assets failure is widely considered as one of the main causes of major accidents in chemical industries such as fires, explosions, and toxic gas releases. Assets criticality analysis is vital to prevent such accidents. Risk-based maintenance (RBM) is among the most advanced comprehensive risk assessment methodologies for the criticality analysis of assets. The present study applies both traditional RBM and Fuzzy RBM (FRBM) methods for the risk analysis of petrochemical assets failure. Four consequence factors comprising operational impact, operational flexibility, maintenance cost, and impact on safety and environment are considered for the risk evaluation of assets failure. Moreover, frequency and risk factor scales are localized for both traditional RBM and Fuzzy RBM methods using an expert panel. The results of the case study show suitability of the FRBM model. Fuzzy numbers show that out of 107 assets, 10 are at the semi-critical level, and the remaining 97 are at the non-critical level. The highest fuzzy risk numbers were obtained for two blowers, where the assets failure value was 99.145. The criticality evaluation results show that the plant in the case study is at the semi-critical level. Given this, it is recommended that risk managers of the plant should customize and prioritise their maintenance planning according to the FRBM value for each asset failure. To this end, maintenance-related recommendations are offered to facilitate and assist decision-makers.

- **Keywords:** Criticality analysis; Decision making; Fuzzy inference system; Risk based maintenance; Petrochemical company; Assets failures

Liyang Ma, Deming Wang, Wenjie Kang, Haihui Xin, Guolan Dou. *Comparison of the staged inhibitory effects of two ionic liquids on spontaneous combustion of coal based on in situ FTIR and micro-calorimetric kinetic analyses*. Pages 326-337.

The inhibitory effects of two ionic liquids (ILs), ethyltributylphosphonium bromide ([P4,4,4,2]Br) and the hydroxyl functional 1-hydroxyethyl-3-methyl imidazolium tosylate ([Hemim]Tos), on spontaneous combustion of coal were investigated and compared. The changes in various active functional groups of coal under IL inhibition were measured by in situ FTIR and analysed semi-quantitatively. Additionally, the impact of the ILs on the heat release rate of coal oxidation was examined by a micro-calorimetric technique. Subsequently, kinetic calculations were employed to elucidate the changes in the intrinsic mechanism of coal oxidation in the presence of ILs. The results revealed that [P4,4,4,2]Br and [Hemim]Tos exhibited distinctive inhibition characteristics on spontaneous combustion of coal. [P4,4,4,2]Br significantly reduced the associative hydroxyl group of coal by destroying the hydrogen bonds and forming stable ether structures. This kind of IL manifested significant inhibition of heat release at the slow oxidation stage of spontaneous combustion of coal. On the other hand, the reductive [Hemim]Tos afforded hydrogen ions from the functionalised OH bonds to eliminate the reactivity of the peroxide radicals. This led to a reduction in the formation of CO double bond intermediates in the transition and rapid oxidation stages at higher temperatures.

- **Keywords:** Ionic liquids; Spontaneous combustion of coal; Staged inhibitory effect; In situ FTIR; Micro-calorimetric kinetic analyses; Inhibiting mechanism

Pezhman Zolfaghari, Mostafa Aghbolaghy, Afzal Karimi, Alireza Khataee. *Continuous degradation of an organic pollutant using heterogeneous magnetic biocatalyst and CFD analysis of the process*. Pages 338-348.

GOx/Fe3O4/TiO2 on natural kissiris support was produced by consecutive preparation of TiO2/kissiris and Fe3O4/TiO2/kissiris followed by immobilization of Glucose Oxidize (GOx). This magnetic biocatalyst was used for continuous elimination of Malachite Green (MG) from aqueous solution in a packed bed reactor through bio-Fenton reaction. The biocatalyst was characterized by FT-IR, EDX and SEM analyses. Residence time distribution (RTD) of MG in the reactor was measured and parameters of the Langmuir-Hinshelwood kinetics model were obtained for the decolorization process. Hydrodynamics of the packed bed reactor were investigated via a thorough computational fluid dynamics (CFD) simulation using Eulerian approach in axisymmetric space and results were validated using experimental RTD curves and decolorization efficiencies. Ultimately, process simulation was utilized to obtain design parameters of the packed bed reactor in recirculating mode with 99.1% decolorization efficiency. The knowledge obtained through this study can be used to design and scale-up continuous and efficient bioreactors for treatment of wastewater.

- **Keywords:** Bio-Fenton; CFD; GOx enzyme; Nanosized magnetite; RTD; Wastewater treatment

Heitor B.S. Bento, Ana K.F. Carvalho, Cristiano E. Rodrigues Reis, Heizir F. De Castro. *Microbial biodiesel production: From sucrose-based carbon sources to alkyl esters via enzymatic transesterification*. Pages 349-356.

Sucrose, in contrast to glucose, is a lower-cost carbon source. This manuscript discloses that its use in submerged fungal growth promotes lipids more suitable to biodiesel production due to lower unsaturation indexes. The wild strain of Mucor circinelloides URM 4182, a potential source of microbial lipid, was grown on three sucrose-based carbon sources: commercial brown sugar, sugarcane juice, and sugarcane syrup, achieving biomass accumulation productivities up to 3.62 ± 0.04 g L^{-1} day^{-1}, and lipid productivities as high as 0.93 ± 0.01 g L^{-1} day^{-1}. Lipid extraction was performed using ethanol, a green alternative to petroleum-derived solvent, and characterized according to their fatty acid distribution, from which C16:0 and C18:1 stand as the most abundant fatty acids. Extracted lipids were converted to ethyl esters via lipase-catalyzed reactions achieving ester contents up to 97.4% and low contents of mono- and diacylglycerols (1.9% and 1.0%, respectively). The interest in utilizing sucrose-based sources is due to the wide abundance of such feedstock in sugarcane-producing regions, and due to the potential of increasing value to these low-cost carbon sources. The results presented herein demonstrate a simple, yet efficient, process of converting sucrose and its derivatives to microbial biodiesel using green-chemistry processes, such as lipid extraction using ethanol, avoiding the use of harsh and toxic chemicals commonly utilized, and enzyme-catalyzed reactions.

- **Keywords:** Sucrose; Sugarcane; Lipase; Microbial lipids; Biodiesel; Mucor circinelloides

Yunfei Zhu, Deming Wang, Zhenlu Shao, Chaohang Xu, Xiaolong Zhu, Xuyao Qi, Fangming Liu. *A statistical analysis of coalmine fires and explosions in China*. Pages 357-366.

Large-scale coalmine accidents have occurred occasionally with great impact on society. To assess the characteristics of large-scale coalmine accidents, a database involving 782 Chinese accidents from 1950 to 2016 was built and analysed. The historical change of large-scale coalmine accidents was divided into four stages according to the accident

number per year. Explosions and fires were the primary causes and deemed to be thermodynamically driven accidents due to their identical thermochemical essence of combustion, interchangeability and producing similar gaseous hazards. By constructing an analysis framework, some useful features were derived from the database. About 55% of the gas explosions occurred in coalmines with low methane-gas emission rates. Coal dust explosions were responsible for about 59% of the fires and explosions with over 100 casualties. The interchangeability of fires and explosions led to 79% of the large-scale coalmine fires and explosions in recent years. As ignition sources, blasting work, self-heating and friction and impact caused 86% of the fires and explosions from 2007 to 2016. About 44% of fires and explosions happened in coalmines with central ventilation systems. About 85% of fires and explosions concentrated on the locations of coalface, heading face and roadway.

- **Keywords:** Fire; Gas explosion; Coalmine; Mine safety; Statistical analysis

Dong Ren, Fang Chen, Zhaogang Ren, Yunwen Wang. *Different response of 17α-ethinylestradiol photodegradation induced by aquatic humic and fulvic acids to typical water matrixes*. Pages 367-373.

Photochemical transformation of steroid estrogens induced by dissolved organic matter has attracted increasing interest due to their extensive presence in natural waters. However, comparative understanding of their photodegradation in aquatic humic acid (HA) and fulvic acid (FA) solutions with different water matrixes is still limited. Herein, 17α-ethinylestradiol (EE2) was selected as a model compound, and photodegraded in riverine water HA and FA solutions as a function of water matrixes to examine the differences in its degradation kinetics and mechanisms. Compared to EE2 photodegradation in HA solution, it was photochemically transformed at a higher rate in FA solution. Quenching experiments revealed that hydroxyl radical was identified as the primary contributor to EE2 degradation in HA solution, while it was a secondary factor in FA solution compared to triplet-state excited species. Due to differential in the predominant mechanisms, EE2 photodegradation in FA solution was promoted in oxygen-poor atmospheres, while an opposite effect was observed for EE2 in HA solutions. The influence of different water matrixes on EE2 photodegradation was clearly different. pH could alter the direct and indirect photolysis of EE2 concurrently, resulting in a constant contribution of the hydroxyl radical, singlet oxygen and triplet-state excited species to EE2 photodegradation. Bicarbonate and chloride ion exhibited no influence on the induced EE2 photodegradation by the HA and FA, while nitrate worked synergistically with HA and FA in accelerating EE2 photodegradation. These findings are helpful for better understanding the photochemical behavior and fate of EE2 in diverse aquatic systems.

- **Keywords:** Photodegradation; 17α-Ethinylestradiol; Dissolved organic matter; Water matrix; Humic substances

Aline L. Arim, Margarida J. Quina, Licínio M. Gando-Ferreira. *Uptake of trivalent chromium from aqueous solutions by xanthate pine bark: Characterization, batch and column studies*. Pages 374-386.

In this study, the performance of chemically modified pine bark for removal of Cr(III) from solutions was investigated. Initially, several chemicals were tested (NaOH, C5H9NO4, H3PO2 and CS2). The xanthate pine bark (XPB) obtained with CS2, was screened as the best adsorbent and thus, it was characterized in respect to morphological and textural properties. Sulfur groups after xanthation reaction were identified on XPB by FTIR and EDS spectroscopies. Equilibrium isotherm and kinetics were determined. The equilibrium data were well described by the Langmuir isotherm allowing to calculate the maximum adsorption capacity (56.5 mg/g). The kinetics is fast and follows a pseudo-second order model. Furthermore, an ion-exchange sorption

mechanism between Cr(III) and Na+ was proposed. Among the desorbing agents tested, the best results were achieved with 2.0 M H2SO4. Moreover, in the column tests, a reduction on the breakthrough time and the stoichiometric time from 36.5 and 22.8%, respectively, was observed, when the feed concentration increased from 230 to 500 mg/L. The breakthrough curves were well modeled by Bohard-Adams, Thomas or Yoon-Nelson equations. Globally, XPB revealed to be a promising adsorbent for uptake Cr(III). The scale-up design and the economic assessment indicated potential applicability for the treatment of real effluents.

- **Keywords:** Cr(III); Biosorption; Xanthation process; Equilibrium; Ion-exchange; Fixed-bed column