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Saikat Sinha Ray, Rohit Kumar Verma, Ashutosh Singh, Suwan Myung, You-In Park, In-Chul Kim, Hyung Kae Lee, Young-Nam Kwon. *Exploration of time series model for predictive evaluation of long-term performance of membrane distillation desalination*. Pages 1-12.

Owing to the inherent complications in membrane distillation (MD) operations, it has become a challenge to acknowledge swiftly and appropriately to safeguard the quality of effluent, particularly when the processing cost is a prominent concern. Membrane wetting in MD operations is a major concern during long-term performance. In this study, machine learning (ML) methodologies were utilized to overcome the limitations of conventional mechanistic modeling. ML applications have never been explored to investigate how operational factors, such as water flux and salt flux, are affected during long-term MD performance. Furthermore, time-dependent factors were neglected, making it difficult to analyze the relationship between effluent quality and operational factors. Therefore, this study demonstrates a novel ML-based framework designed to enhance the performance of MD. The ML-based framework consists of an autoregressive integrated moving average (ARIMA) and utilizes a unique pathway to explain the impact of time series among operational factors. The accuracy of forecasting has been explored by utilizing 180 h (180 datasets), that was further used and divided into training (165 datasets) and test datasets (15 datasets). Eventually, the ARIMA model demonstrated a highly precise relationship order between the model and experimental data, which can be further used to forecast membrane performance in terms of wetting and fouling. The selected ARIMA model (3,2,1) appears to be an adequate model for water and salt flux data which has been effectively used to capture the course of permeate water and salt flux by producing the smallest forecast RMSE. The RMSE values were observed to be 0.22 and 0.05 for water and salt flux respectively, which can better predict long time series with high frequency. These frameworks can be applied for the early prediction of membrane wetting if ample high-resolution data are available.

- **Keywords:** Water treatment; Membrane distillation; Time series; Machine learning; Predictive analysis

Yingying Wang, Yuqi Li, Feng Yin, Wentao Wang, Haibo Sun, Jianchang Li, Ke Zhang. *An intelligent UAV path planning optimization method for monitoring the risk of unattended offshore oil platforms*. Pages 13-24.

To ensure the safe operation of static and dynamic devices in a limited platform space and prevent security threats caused by accidents and external intruders, the unmanned

aerial vehicle (UAV) is becoming an important tool to monitor and reduce the operational risk of unattended offshore oil platforms. However, UAVs may encounter location errors, adversely affecting patrol efficiency and accuracy. Therefore, the optimal UAV path planning is vital to ensure complete monitoring routes and reduce the risk presented by the marine environment, devices, and employees on unattended offshore platforms. This paper established a multi-objective mathematical model with the shortest flight path and minimum correction times for the intelligent UAV patrol of unattended offshore platforms. An intelligent algorithm with large-scale constraints for UAV path planning was proposed based on non-dominated sorting genetic algorithms. A flight path length of 8076.11 m and 25 correction times presented the optimal solution. The results indicated that the proposed algorithm could be used to plan an effective and accurate three-dimensional (3D) UAV flight path according to the size of the offshore oil platform. This is highly significant for the intelligent risk monitoring of unattended offshore platforms in practical engineering in the future.

- **Keywords:** Unattended offshore platform; Flight path planning; NSGA-II; Error correction; Genetic operator

Jandira Leichtweis, Yasmin Vieira, Nicoly Welter, Siara Silvestri, Guilherme Luiz Dotto, Elvis Carissimi. *A review of the occurrence, disposal, determination, toxicity and remediation technologies of the tetracycline antibiotic*. Pages 25-40.

Tetracycline (TC) is a group of antibiotics that includes chlorotetracycline (CTC), doxycycline (DC), and oxytetracycline (OTC). TC is the secondary most used antibiotic worldwide to treat diseases caused by bacteria. It is noteworthy that in the human and animal metabolic processes, about 60% and 17–80% of the TC dosage administered are not adsorbed and are excreted in urine and feces. Its widespread use in human and veterinary treatments is leading to the situation of environmental contamination, both in soil, surface, and underground waters. The first two sections of this review paper present an overview of the problem of water and soil contamination, and the situation on the worldwide use of TC. The third section focuses on analytical methods for detecting TC in the most diverse types of samples. Furthermore, in the following chapters it is discussed TC toxicity and the application of chemical, physical, and biological processes in removing TC in wastewater. At last, hybrid and emerging technologies for TC degradation as an environmental contaminant are presented, and some future challenges that must be faced by this research field are summarized. A critical analysis from the authors' perspective is presented at the end of each session.

- **Keywords:** Pharmaceuticals; Hazardous pollutant; Analytical techniques; Environmental remediation

Maria Molinos-Senante, Alexandros Maziotis. *Prediction of the efficiency in the water industry: An artificial neural network approach*. Pages 41-48.

The measurement of efficiency of water utilities has been traditionally carried out using econometric methods or linear programming techniques. Alternatively, in this study a data mining non-parametric method is used, such as an artificial neural network (ANN) approach, to predict the efficiency of several water companies in England and Wales. The further use of a regression tree model allowed us to visualize and quantify the impact of operating characteristics on efficiency. The average efficiency score for the water industry was 0.411. Average scores for water only companies and water and sewerage companies were 0.210 and 0.626, respectively. Only one water company was identified as being fully efficient. This indicates that most of the English and Welsh water companies need to make substantial improvements in their managerial practices to

catch-up with the most efficient ones in the industry. Several operating characteristics such as water leakage, water taken from different sources and population density were found to influence efficiency. The percentage of water leakage was identified as the most relevant operational variable influencing the efficiency of water companies. The findings of our study aim to support benchmarking analysis in regulated industries and to get a better insight on what drives efficiency.

- **Keywords:** Artificial neural networks; Data envelopment analysis; Regression tree; Efficiency measurement; Environmental variables; Water utilities

Yup Yoo, Jonghun Lim, Juwon Lee, Junghwan Kim, Hyungtae Cho. *Optimization of explosive fumes ventilation layout in vacuum pressure impregnation process*. Pages 49-61.

Vacuum pressure impregnation (VPI) is a primary process by which epoxy resin is impregnated into the stator windings of large generators and motors to enhance their physical properties. However, the vaporization of epoxy resin generates hazardous resin fumes during the VPI process, and the residual fumes leak into the atmosphere. This leakage is a safety and environmental hazard in the workplace as it can cause fire, explosion, and respiratory diseases. Therefore, it is crucial to reduce the hazard by designing an optimal ventilation system. This study proposed optimization of the explosive fumes ventilation Layout in the VPI process using computational fluid dynamics (CFD). A total of 12 Layouts of the ventilation system was designed according to the air inlet and outlet positions. This investigation used the pseudo transient method and the RNG k–ε turbulence model. An optimal Layout with the highest ventilation efficiency and the shortest LEL arrival time was determined through CFD analysis. In the optimal Layout, the LEL arrival time was 372 s, down about 59% from the model presented in the previous study, and the ventilation efficiency was the highest at 0.962.

- **Keywords:** Computational fluid dynamics; Ventilation system; Resin fume; Vacuum pressure impregnation (VPI)

Yanli Fu, Ying Zhu, Hao Dong, Jing Li, Weiyi Zhang, Yingying Shao, Yanqiu Shao. *Mechanisms of the effects of humic acid on antibiotic resistance genes and microbial communities in Cd-contaminated soils*. Pages 62-69.

Humic acid (HA) is an organic macromolecular compound that widely exists in nature, but its effect on antibiotic resistance genes (ARGs) in Cd-contaminated soil is unknown. This study investigated the effects of Cadmium (Cd) and HA in soil on ARGs, mobile genetic elements (MGEs), and bacterial communities. The relative abundance of ARGs and MGEs increased 0.89-fold and 1.12-fold after the addition of 2 mg kg−1 Cd to the soil, and 1.06-fold and 1.68-fold after the addition of 8 mg kg−1 Cd. Redundancy analysis further revealed that among environmental factors, available Cd was the dominant factor influencing ARGs. In Cd-contaminated conditions, the addition of high concentrations of HA suppressed the expression of ARGs and MGEs. The abundance of ARGs and MGEs decreased by 0.12-fold and 0.44-fold after the addition of HA (50 mg kg−1) to the soil at a Cd concentration of 2 mg kg−1, and by 0.18-fold and 0.41-fold at a Cd concentration of 8 mg kg−1. IntI1 was significantly associated with all ARGs (sul1, sul2, tetG, tetW), and intI2 was significantly correlated with most ARGs (sul2, tetG, tetW). Network analysis illustrated that Proteobacteria were the main host bacteria causing changes in the abundance of ARGs and MGEs. HA has an important role in agricultural production. To reduce the enrichment of ARGs in Cd-contaminated soil, the addition of higher concentrations of humic acid can be considered to mitigate the environmental and biological hazards.

- **Keywords:** Humic acid; Resistance gene abundance; Microorganisms; Environmental factors

Xudong Zheng, Wen Sun, Ang Li, Yuzhe Zhang, Zhongyu Li. *Bacterial cellulose nanofibrous ion imprinted aerogel for highly efficient recognition and adsorption of Dy(III)*. Pages 70-79.

The highly selective recovery of Dy(III) from used rare earth products has high environmental and economic benefits. In this paper, biocompatible bacterial cellulose with a unique 3D network structure was used as the basic structure, graphene oxide and polyethylene glycol were introduced to increase the adsorption capacity, and the ion imprinting technology was used to prepare a green aerogel that could adsorb dysprosium ions with a high selectivity. The various properties of aerogels were characterized by SEM, FT-IR and BET. Experiments proved that the introduction of graphene oxide and polyethylene glycol brought a higher stability and repeatability to aerogel, and the introduction of a large number of carboxyl groups also promoted the effective coordination of aerogel with dysprosium. Adsorption experiments showed that I-GO-OBC-pDA-PEG aerogel could effectively adsorb dysprosium, and its maximum adsorption capacity for Dy(III) was 49.904 mg g−1, and its maximum adsorption capacity was 10 mg g−1 higher than that of the non-imprinted aerogel, which was a good proof of the effectiveness of the ion imprinting technology. The repeatability test showed that after five adsorption-desorption cycles, the adsorption capacity of the imprinted aerogel was maintained at about 80% of the maximum adsorption capacity. All results showed that I-GO-OBC-pDA-PEG aerogel could efficiently recover dysprosium ions.

- **Keywords:** Bacterial cellulose; Ion imprinted; Aerogel; Dysprosium; Selective adsorption

Ya-Ping Yang, Jun-Cheng Jiang, An-Chi Huang, Yan Tang, Ye-Cheng Liu, Lin-Jie Xie, Chuan-Zhu Zhang, Zhi-hao Wu, Zhi-Xiang Xing, Fei Yu. *3-(Trifluoromethyl)benzoylacetonitrile: A multi-functional safe electrolyte additive for LiNi0.8Co0.1Mn0.1O2 cathode of high voltage lithium-ion battery*. Pages 80-90.

The high nickel layered oxide cathode LiNi0.8Co0.1Mn0.1O2 (NCM811) is widely used in new energy power and equipment due to its high density and low cost. However, the NCM811 cathode is prone to structural rupture, dissolution of transition metal ions, and damage to the electrode/electrolyte interface under high voltage, causing degradation of battery performance and safety issues. In this paper, 3-(Trifluoromethyl)benzoylacetonitrile (3-TBL) was selected as a film-forming flame-retardant additive for the NCM811 cathode of the high-voltage lithium-ion battery, and the synergistic effect with lithium difluoro(oxalato)borate enhanced the battery cycle and safety performance. The results show that: 3-TBL is oxidized preferentially more than carbonate solvent to form a stable and dense cathode-electrolyte interface film, which effectively prevents the continuous oxidative decomposition of the electrolyte and enhances the rate of cycling and overcharge resistance of the Li/NCM811 cells under high pressure. Furthermore, the 3-TBL modified electrolyte can also delay the thermal decomposition temperature of the commercial electrolyte and improve its flame retardant properties. Kinetic analysis showed that the additive increased the activation energy required for the thermal decomposition reaction of electrolyte and NCM811 cathode mixture. Therefore, the additives 3-TBL improve the intrinsic safety of the electrolyte and electrolyte interface, providing a feasible idea for the development of high energy density and high safety electrolytes.

- **Keywords:** High voltage Lithium-ion battery; NCM811 cathode; Electrolyte additives; 2-Cyano-3'-(trifluoromethyl)acetophenone; Interfacial properties; Safety performance

Ye-Cheng Liu, Jun-Cheng Jiang, An-Chi Huang, Yan Tang, Ya-Ping Yang, Hai-Lin Zhou, Juan Zhai, Zhi-Xiang Xing, Chung-Fu Huang, Chi-Min Shu. *Hazard assessment of the thermal stability of nitrification by-products by using an advanced kinetic model*. Pages 91-101.

Since the 1990 s, sporadic explosion accidents have occurred in the chemical industry. Accidents related to nitrification reactions or nitrification substances have had the most severe consequences. One reason for this phenomenon is the high risk of nitrification by-products, which are liable to combust and explode. Special attention must be paid to the production, collection, storage, and disposal of nitrification by-products. This study examined the thermal stabilities of the phenolic by-products created during nitrobenzene formation. The thermal stabilities of three representative aromatic nitrophenol by-products were determined using differential scanning calorimetry, accelerating rate calorimetry, and thermogravimetric analysis. Advanced thermodynamic models were established for calculation and fitting, which provided reliable data support for exploring the intrinsic stability of nitrification by-products.

- **Keywords:** Nitrification by-product; Thermal stability; Differential scanning calorimetry; Thermodynamic model; Intrinsic stability

Jean A. Barbosa, Christian J.R. Coronado, José C. de Andrade, Celso E. Tuna, Marcos H. Silva, João A. Carvalho Junior, Andrés Z. Mendiburu. *Experimental determination of upper flammability limits of synthesized iso-paraffins (SIP), Jet fuel and their mixtures with air at atmospheric and sub-atmospheric pressures*. Pages 102-115.

Synthesized iso-paraffins (SIP) are compounds that can be blended with traditional aviation fuels up to 10% vol. to reduce greenhouse gas emissions. The safety properties of these fuels need to be determined to guarantee their reliable utilization. These properties include the upper flammability limit (UFL). The objective was to determine experimentally the UFL in air of SIP, jet fuel, and mixtures containing 10% (F10) and 50% (F50) of SIP on a mass basis, respectively. The initial conditions involved different initial temperatures and pressures. The experimental configuration followed the ASTM E681 standard. The temperature range was from 420 to 470 K and the pressure range was from 101.3 kPa to 20 kPa. The results show that the UFLs of the tested compounds have a second-order tendency with respect to pressure and constant temperature. The F10 mixture has a significant reduction of the UFL at 20 kPa. The experimental results were fitted by using regression models and empirical correlations which allow the determination of UFLs at different initial temperatures and pressures.

- **Keywords:** Farnesane (SIP); Jet fuel; Upper flammability limit; Pressure dependence; Pre-mixed flames

Mengyuan Zou, Weijun Tian, Jing Zhao, Meile Chu, Tiantian Song. *Quinolone antibiotics in sewage treatment plants with activated sludge treatment processes: A review on source, concentration and removal*. Pages 116-129.

According to the existing research results, this paper reviews the influent and effluent concentrations, migration and transformation, and influencing factors of quinolone antibiotics in sewage treatment plants (STPs) with activated sludge treatment processes. Animal breeding and slaughtering wastewater, pharmaceutical wastewater and medical

and domestic sewage may be the main sources of quinolone antibiotics. The compounds and concentrations of quinolone antibiotics in influents and effluents around the world are quite different, which is generally due to the difference in social and environmental factors in different regions, and the different treatment processes and operating parameters adopted. The migration and transformation of quinolone antibiotics is usually the result of the synergistic effect of sludge adsorption, biodegradation and photolysis. Sludge adsorption based on electrostatic interaction, hydrophobic forces and other mechanisms is the dominant route to remove quinolone antibiotics, but it does not reduce the total amount of the target antibiotics. An appropriate selection of conditions and control of process variables are beneficial to improve the removal of quinolone antibiotics by biodegradation with co-metabolism. Sources control, treatment processes improvement, fate understanding and prediction, monitoring strategies and risks assessment are potential options for improving the elimination and controlling the pollution of quinolone antibiotics in the future.

- **Keywords:** Sewage treatment plant; Quinolone antibiotics; Concentration; Removal efficiency; Migration; Transformation

Asma Nasrullah, Amir Sada Khan, Shahan Zeb Khan, Abrar Inayat, Taghreed M. Fagieh, Esraa M. Bakhsh, Kalsoom Akhtar, Sher Bahadar Khan, Israf Ud Din. *Kinetics and thermodynamic study of Calligonum polygonoides pyrolysis using model-free methods*. Pages 130-138.

Pyrolysis kinetics was carried out for Calligonum polygonoides (C. Polygonoides) in an inert atmosphere at three different heating temperatures such as 10, 15, and 20 °C/min using thermogravimetric analysis. Physicochemical properties were studied using bomb calorimeter, elemental analyzer, and Fourier Transform Infrared Spectroscopy. C. Polygonoides have a calorific value of 16.33 MJ/kg. Gas chromatography–mass spectrometry was used to identify gases produced during pyrolysis. Thermogravimetric analysis was used to investigate the pyrolysis characteristics of biomass. Activation energy for the three zones of pyrolysis were determined using Kissinger and Ozawa model-free methods. Activation energy calculated for zone I, zone II and zone III using Ozawa and Kissinger model was 133.73, 164.50, 254 KJ/mol and 135.61, 165.88, and 253.00 KJ/mol, respectively. Thermodynamic parameters such as enthalpy, entropy, and Gibbs free energy were calculated for the three different zones. Kinetic and thermodynamic study confirmed that C. Polygonoides can be used as useful and potential bioenergy feedstock.

- **Keywords:** Biomass; Thermogravimetric analysis; Kinetics parameters; Pyrolysis; Kinetics models

La Ta, Zhilei Wang, Bin Zhang, Yiming Jiang, Yunyu Li, Qingyuan Wang, Tao Zhang, Min Hua, Xuhai Pan, Juncheng Jiang. *Experimental investigation on shock wave propagation and self-ignition of pressurized hydrogen in different three-way tubes*. Pages 139-152.

This paper experimental investigated the shock wave propagation characteristics and self-ignition produced by the high-pressure hydrogen release in the three-way tubes. Two Y-shaped tubes (60°, 120°) and one T-shaped tube (180°) were used in the experiments and the initial release pressure was 3–8 MPa. The pressure and photoelectric signals in tubes were recorded by the sensor. The results showed that the intensity of shock wave was enhanced or attenuated during the entire releasing process, but the dominant effect was distinct under different conditions and the two effects synergistically affected the occurrence possibility of self-ignition. The critical release pressure for self-ignition in the three-way tubes decreased with the increasing of the bifurcation angle, and the most difficult to occur the self-ignition was the 60° Y-tube in

this study. In addition, quenching occurred in the 60° Y-tube when the initial release pressure was 6 MPa, because the temperature of the mixture dropped by the expansion effect. Furthermore, the intensity of the reflected shock wave was not strong enough to promote hydrogen rekindled. This experimental results have reference value for the safety of high-pressure hydrogen production, storage and transportation, and are helpful to understand the influence of bifurcation structure on self-ignition in energy application.

- **Keywords:** Hydrogen safety; Pressurized hydrogen; Spontaneous ignition; Bifurcation structures; Shock wave

Chandra M.R. Vendra, Ashish V. Shelke, Jonathan E.H. Buston, Jason Gill, Daniel Howard, Elliott Read, Ahmed Abaza, Brian Cooper, Jennifer X. Wen. *Numerical and experimental characterisation of high energy density 21700 lithium-ion battery fires*. Pages 153-165.

High energy density lithium-ion batteries (LIBs) are well suited for electrical vehicle applications to facilitate extended driving range. However, the associated fire hazards are of concern. Insight is required to aid the development of protective and mitigation measures. The present study is focused on 4.8 Ah 21700 cylindrical LiNixCoyMnzO (NMC) LIBs at 100% state of charge (SOC) with the aim to develop a viable predictive tool for simulating LIB fires, quantifying the heat release rate and temperature evolution during LIB thermal runaway (TR). To aid the model development and provide input parameters, thermal abuse tests were conducted in extended volume accelerating rate calorimetry (EV-ARC) and cone calorimetry. Some cells were instrumented with inserted temperature probe to facilitate in-situ measurements of both cell internal and surface temperatures. The mean peak values of the heat release rate, cell surface and internal temperatures were experimentally found to be 3.6 kW, 753 °C and 1080 °C, respectively. An analytical model has been developed to predict cell LIB internal pressure evolution following vent opening. The model uses the measured cell internal temperature and EV-ARC canister pressure as input data. Its predictions serve as boundary condition in the three-dimensional computational fluid dynamics (CFD) simulation of TR induced fire using opensource code OpenFOAM. The predicted transient heat release rate compare favourably with the measurements in the cone calorimetry tests. Predictions have also been conducted for an open cluster to assess the likelihood of TR propagation in the absence of cell side rupture. The present modelling approach can serve as a useful tool to assess the thermal and environment hazards of TR induced fires and aid design optimisation of mitigation measures in enclosed cell clusters/modules.

- **Keywords:** 21700 Lithium-ion battery; Cell internal pressure and temperature evolution, Venting of flammable gases; Fire simulation; Computational Fluid dynamics (CFD); Safety

Mohamed G. Gado, Mohamed Nasser, Ahmed A. Hassan, Hamdy Hassan. *Adsorption-based atmospheric water harvesting powered by solar energy: Comprehensive review on desiccant materials and systems*. Pages 166-183.

Atmospheric water harvesting has been inexorably proliferated as a potential source of freshwater, notably for remote areas that lack access to water and electricity. This technology could be significantly operated with renewable energy sources. The current study comprehensively reviews the state-of-the-art atmospheric water harvesters and their desiccant materials. Firstly, a detailed survey on desiccant materials, silica gel, Metal-organic frameworks (MOFs), hydrogels, zeolite, hygroscopic salts and composite desiccant materials is illustrated. The review particularly focuses on the materials adsorption capability, kinetics, proper matching with climate conditions. Moreover, the most suitable adsorbents are thoroughly surveyed for a wide range of climate conditions,

especially for water scarcity regions (i.e., arid zones) that are characterized by low relative pressures. Moreover, various designs of solar-powered atmospheric water harvesters are comparatively summarized, including fixed and portable installations. It can be concluded that MOF-801, MOF-808, MOF-841, HKUST-1, and CPO-27(Ni) have a superior potential for water harvesting in arid areas. Additionally, MIL-101(Cr) has superior water uptake and kinetic at high relative pressure (i.e., humid areas), and it is irrelevant for water harvesting at dry zones. It is found that the cost of the collected water from atmospheric water harvesting technology is about 0.062–0.86 $/kg of adsorbent. This work provides beneficial perspectives for selecting the most relevant desiccant materials beside the appropriate solar system for water harvesting applications.

- **Keywords:** Adsorption water harvesting; Desiccant materials; Solar-powered water harvesting systems; Host materials; Hygroscopic salts; MOFs

Hong Lin, Haochen Luan, Lei Yang, Chang Han, Hassan Karampour, Guoming Chen. *A safety assessment methodology for thermo-mechanical response of offshore jacket platform under fire*. Pages 184-198.

Fire accidents caused by the leakage of combustible gas pose a serious threat to the offshore platform, probably resulting in local damage and even progressive collapse of the platform structure. The aim of this paper is to systematically assess the structure safety of platform under fire accidents. The uniqueness of this study is the integration of fluid-thermal-structural coupling simulations with the advantage of considering an accidental fire scenario. The dispersion behavior of leaked gas is studied and the development of elevated temperature generated on the offshore platform during the combustion process is predicted based on Computational Fluid Dynamics (CFD)- Finite Element Analysis (FEA) coupling method. Then, the thermal-mechanical coupling analysis is performed to predict the responses of structure under high temperature. Eventually, the criteria of ultimate bearing capacity of the component and the overall offshore structure are utilized to evaluate the safety of the offshore platform. The results show that with the development of fire, the high temperature zone spreads to cover the space between two neighboring decks, and the maximum temperature in the platform reaches 877 °C. The structural strength of the platform is significantly affected by high temperature. Under the vertical load, the ultimate bearing capacity of the platform at high temperature is decreased by 78% compared to that at ambient temperature. The methodology proposed could be applied to the safety assessment of other similar offshore or marine facilities, so as to support to the process safety in fire accidents.

- **Keywords:** Offshore jacket platform; Fire accidents; Fluid-thermal-structural coupling analysis; Thermo-mechanical response; Safety assessment

Xiaonuo Zhang, Chaoyang Huang, Jie Ren, Tadiyose Girma Bekele, Hongxia Zhao. *Effect of cyclodextrin on desorption of petroleum hydrocarbons in soil*. Pages 199-208.

The present study delineated to explore the possibility of using cyclodextrins as an environmentally friendly solubilizer for enhancing the desorption efficiency of petroleum hydrocarbons (PHs) in the contaminated soil. The results showed that cyclodextrins could promote the transfer of PHs from the soil solid phase to the aqueous phase. Through the batch desorption experiments, single-factors influencing the desorption efficiency, including desorption time, species of cyclodextrin, solid to liquid ratio (S/L ratio) of soil to solvent, concentrations of solubilizer and concentrations of the contaminated soil were investigated. In addition, the response surface methodology analysis were used to identify the optimal desorption conditions, and the optimal desorption parameters were concluded as the follows: desorption time of 34 h, S/L ratio of soil to solvent of 1:25,

concentration of β-CD of 0.75 g/L (for PAHs), desorption time of 18 h, S/L ratio of soil to solvent of 1:5, concentration of β-CD of 4.8 g/L (for n-alkanes). The highest desorption efficiency of two representative PHs, polycyclic aromatic hydrocarbons (PAHs, phenanthrene, fluoranthene and pyrene) and n-alkane (C16, C20, C24, C28 and C32), were 63.0% and 61.7%, respectively. This study presented new-positive evidence of cyclodextrins for enhancing desorption of PHs, was of great importance for enhancement of bioavailability of PHs, and further revealed the great potential of cyclodextrins as a solubilizer in-situ assisting removal of PHs in the petroleum-contaminated sites.

- **Keywords:** Petroleum hydrocarbons; Cyclodextrin; Desorption; Soil remediation

Xi Cui, Bingbing Jia, Fengwei Diao, Xue Li, Jing Xu, Zhechao Zhang, Frank Yonghong Li, Wei Guo. *Transcriptomic analysis reveals the molecular mechanisms of arbuscular mycorrhizal fungi and nitrilotriacetic acid on Suaeda salsa tolerance to combined stress of cadmium and salt*. Pages 210-220.

Halophytes are dominant plants in the phytoremediation of heavy metal contaminated saline soils. Arbuscular mycorrhizal (AM) fungi can improve plant abiotic stress tolerance and chelating agents nitrilotriacetic acid (NTA) can alleviate heavy metal stress. However, the combined effects and mechanisms of two amendments on halophytes grown in heavy metal contaminated saline soils are largely unknown. Pot experiment was conducted to explore the molecular mechanisms of Funneliformis mosseae (Fm) and NTA (10 mmol·kg−1) on Suaeda salsa tolerance to combined stress of Cd (5 mg·kg−1) and NaCl (2.5 g·kg−1). The results showed that AM fungi and NTA promoted growth of S. salsa, increased accumulations of Na+, Cd and mineral elements, but decreased Na+, Cd and malondialdehyde (MDA) concentrations in shoots under combined stress. Transcriptomic analysis presented various regulation pathways of the single or combined application of AM fungi and NTA on S. salsa. The identified differentially expressed genes (DEGs) in (Fm+NTA)/CK were mainly involved in antioxidant defense, osmoregulation, and photosynthesis; the DEGs in (Fm+NTA)/Fm were related to the maintenance of the cell membrane integrity and plant abiotic stress tolerance; and the DEGs in (Fm+NTA)/NTA were related to the enhancement ability of secondary cell wall synthesis and transcription factor. Our study provides new insights into the molecular mechanisms of AM fungi and NTA on halophytes tolerance to combined stress of heavy metal and salt.

- **Keywords:** Halophyte; Hormonal regulation; Nitrogen metabolism; Arbuscular mycorrhizal fungi; NTA; Transcriptome

Khaled Elmaadawy, Bingchuan Liu, GK Hassan, Xiaohe Wang, Qiuwei Wang, Jingping Hu, Huijie Hou, Jiakuan Yang, Xiaolong Wu. *Microalgae-assisted fixed-film activated sludge MFC for landfill leachate treatment and energy recovery*. Pages 221-231.

The sustainability and innovation of a novel leachate treatment technology is a matter of vital significance. Bio-electrochemical-driven wastewater and leachate treatment methods, particularly MFC, and their improvements have attracted scientists' attention recently. This study developed a new MFC system, which consisted of an anodic chamber, a cathode chamber with fixed biofilm carriers and a low-cost sheet of carbon felt between them as a membrane-like separator. The study was conducted to evaluate the capacity of MFC coupled with integrated fixed-film activated sludge (IFAS), to enhance the efficiency of the treatment and the amount of energy produced. Three MFC systems with different cathode processes were compared, namely, conventional activated sludge (MFC-AS), MFC-IFAS, and microalgae coupled MFC-IFAS (MFC-IFAS/MA). The experimental results revealed that MFC-IFAS/MA produced higher power density and nitrogen removal than the other two systems. The average removals of COD, NH4+-N,

and total nitrogen (TN) were, 69.9%, 84.2% and 60.5% for MFC-AS, 84.3%, 79.2% and 71.6% for MFC-IFAS; and 82.0%, 90.3% and 88.6% for MFC-IFAS/MA. MFC-IFAS/MA demonstrated its superior electrochemical behaviors and nitrogen removal and this behavior was referring to the dual effect of fixed-biofilm and microalgae assimilation. This study investigated for the first time the symbiosis between microalgae and IFAS in an MFC reactor, which may open a new prospect for MFC application.

- **Keywords:** Microbial fuel cell; Microalgae; Carbon felt separator; Integrated fixed activated sludge; Microbial community

Yinan Yang, Jun Li. *Investigation of macro-kinetics of coal-oxygen reactions under varying oxygen concentrations: Towards the understanding of combustion characteristics in underground coal fires*. Pages 232-241.

The typical combustion mode of underground coal fires (UCFs) is smoldering during which the reaction zone is not exposed to a constant oxygen concentration. Understanding the macro-kinetics of coal-oxygen reactions under varying oxygen concentrations, especially the extremely oxygen-depleted condition, is of both theoretical importance and practical relevance to the control and extinguishment of UCFs. Considering the actual conditions of UCFs, thermal analysis tests under four oxygen concentrations (from 21% to 3%) and three heating rates (1, 2 and 5 °C /min) were carried out. Thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) results were obtained for a bituminous coal sample from Inner Mongolia, China. With the global reaction assumption, the macro-kinetics parameters (the apparent activation energy, the pre-exponential factor and the kinetics model function) were determined. On the profiles of the apparent activation energy (Ea), three peak values were observed, physically interpreted as the depletion of volatiles, the formation of plastic mass and the depletion of char, respectively. This interpretation was verified by characteristic temperatures extracted from the experimental data. With the decrease of the oxygen concentration from 21% to 9%, two peak values diminish gradually. The case with 3% oxygen concentration gives a nearly monotonically declining Ea, indicating that under that particular condition, oxygen diffusion stands as the only limiting factor across all stages of coal-oxygen reactions. The best-fit kinetics model functions suggest that the char oxidation stage falls into the kinetics-controlled regime when the oxygen concentration is as low as 9%. For the volatiles burning stage, the universal ignition index (Fz) is found to be effectively related to the reaction regime for a variety of coal ranks. The quantitative results obtained can be integrated into any CFD multi-physics models as a sub-model for chemical kinetics.

- **Keywords:** Underground coal fires; Coal-oxygen reactions; Macro-kinetics; Oxygen concentration; Thermal analysis; Kinetics triplet

Chunbo Pang, Dawei Duan, Zhiying Zhou, Shangbo Han, Longchao Yao, Chenghang Zheng, Jian Yang, Xiang Gao. *An integrated LSTM-AM and SPRT method for fault early detection of forced-oxidation system in wet flue gas desulfurization*. Pages 242-254

Safe and efficient operation of the forced-oxidation system is of importance to the wet flue gas desulfurization (WFGD). However, equipment and system failures are commonly found due to the long-time running, frequent blower switching, and heavy workload etc., especially after the ultra-low emission (ULE) renovation to meet strict emission standard in China. This work develops a fault early detection method to improve the predictive maintenance of the forced-oxidation system including blowers, pipes, and the slurry tank. A model based on long short-term memory (LSTM) network and attention mechanism (AM) is constructed to predict real-time operation parameters and compare with the

measured values. Then the sequence probability ratio test (SPRT) is utilized to analyze the prediction-measurement residual and provide automatic and dynamic warning. All the data for model training and prediction are from the build-in distributed control system (DCS) without additional sensors. The LSTM-AM model proves to accurately predict time-dependent and highly relevant parameters. SPRT can sensitively perceive the fault-caused residual deviation while alleviating the noises. Industrial application to the cases in a 50 MW combined heat and power generation plant is then carried out. Results show that the bearing failure of the oxidation blower and branch pipes (immersed in the slurry tank) blockage can be forecast in advance when the incipient degradation occurs.

- **Keywords:** Fault early detection; Forced-oxidation system; Long short-term memory network; Attention mechanism; Sequential probability ratio test

Ana Rita Ferreira, Lars Breinholt, Kamilla M.S. Kaarsholm, Diego Francisco Sanchez, Ravi K. Chhetri, Jens Muff, Henrik R. Andersen. *Feasibility study on produced water oxidation as a pretreatment at offshore platform*. Pages 255-264.

Produced water (PW) generated worldwide has lately become an issue of environmental concern. PW has a complex composition and a suitable treatment at offshore oil and gas platforms is required to achieve zero harmful discharge into the sea. The feasibility of electrochemical oxidation, heat-activated persulfate and ozonation was investigated as PW pretreatment. For comparison purposes, a common oxidant dosage level of 5% and 10% treatment equivalent chemical oxygen demand(COD) removal were established. Aiming to access PW biodegradability, an assay for biological oxygen demand(BOD) for high salinity matrix was also developed as a tool to characterize treatment efficiency. Electrochemical oxidation was largely independent on the anode materials, and controlled by the applied charge passed through the system. Heat-activated persulfate reaction was time-consuming and dependent on activation temperature, as well as initial oxidant concentration. Both methods reduced COD and BOD without significantly improving PW biodegradability, probably due to by-products generation. Ozonation had the most promising results applying doses ranging from 3.5 to 151mgO3/L. The benzene in PW after ozonation reduced up to 71% alongside with> 70% toxicity reduction for tested doses. Ozonation also showed to marginally improve PW biodegradability, which underline the potential of ozone to facilitate a subsequent biological treatment.

- **Keywords:** Offshore produced water; Chemical oxidation process; Electrochemical oxidation; Ozonation; Heat-activated persulfate

Lijuan Liu, Zhangqiang Dong, Dongyang Qiu, Jiashun Hao, Xianfeng Chen, Chuyuan Huang. *Effect of powder inhibitors on ignition sensitivity evolution of wood-plastic mixed dust: Based on thermal decomposition behavior and deflagration residues*. Pages 265-273.

The ignition temperature (IT) of the dust cloud is one of the main parameters of combustible dust deflagration risk assessment. Since the previous research focuses on the IT of single dust, in order to reduce the deflagration risk of mixed dust, the effects of dust concentration and dispersed pressure on the IT of wood-plastic mixed dust and the inhibition effects of different powder inhibitors were investigated through experiments. The thermal decomposition behavior of the mixed dust was studied by comprehensive thermal analysis, and the surface characteristics of the deflagration products were analyzed by FTIR spectra, thus revealing the inhibition mechanisms of inhibitors on ignition sensitivity of mixed dust. The results showed that the best ignition conditions for wood-plastic mixed dust were 300 g/m3 and 15 kPa. Ammonium polyphosphate (APP) and aerosil had significant inhibition effects on the ignition sensitivity of wood-plastic mixed dust, and the inhibition effect was better with the increase of inerting ratio. Their

inhibition mechanisms are different, and the inhibition effect of APP is better. It was worth noting that APP can promote the initial decomposition of wood-plastic mixed dust, resulting in accelerated dehydration and carbonization rate of mixed dust and improved thermal stability.

- **Keywords:** Wood-plastic mixed dust; Ignition temperature; Inhibition effect; Inhibition mechanism

Bing Wang, Yuanyuan Zhu, Dinglin Li, Chao Wu. *Evidence-based accident prevention and its application to hazardous chemical storage accident prevention*. Pages 274-285.

Many accidents occur owing to decision-making failures in accident prevention. From an information perspective, decision-making failures in accident prevention are due to a lack of necessary information. Moreover, the research–practice gap is a long-standing and common problem in accident prevention. To solve the abovementioned problems to improve accident prevention, this study proposes a new accident prevention approach referred to as evidence-based accident prevention. This approach emphasizes the use of the best accident prevention evidence in the accident prevention decision-making process. It is regarded as a practical approach to avoid the lack of safety information to improve the quality of accident prevention decision-making and narrow the research–practice gap vis-à-vis accident prevention. First, this paper explains that evidence-based accident prevention is based on accident prevention failures from a safety information perspective. Second, this study proposes a model for evidence-based accident prevention. Finally, this study applies an evidence-based accident prevention approach to the prevention of hazardous chemical storage accidents in a paint manufacturing plant in Tianjin, China, as a case study. This study aims to help researchers and practitioners to understand the evidence-based accident prevention approach and lay a foundation for the future study and practice of evidence-based accident prevention.

- **Keywords:** Evidence-based approach; Accident; Accident prevention; Evidence-based accident prevention; Decision-making in accident prevention; Hazardous chemical storage accident

Luciana de Melo Pirete, Franciele Pereira Camargo, Guilherme M. Grosseli, Isabel K. Sakamoto, Pedro S. Fadini, Edson Luiz Silva, Maria Bernadete Amâncio Varesche. *Influence of ethanol and nitrate on ibuprofen removal in batch reactors under denitrifying conditions*. Pages 297-309.

The optimized removal of the anti-inflammatory drug ibuprofen inoculated with activated sludge biomass in batch reactors was evaluated, using the variables ibuprofen (60 – 80 μg L-1), ethanol (130 – 230 mg EtOH L-1) and nitrate (130 – 230 mg NO3- L-1) by rotational central compound design. A higher removal efficiency of ibuprofen (97.5 ± 3.1%) was observed with 95.9 mg NO3- L-1, 109.9 μg IBU L-1 and 110.6 mg EtOH L-1. Under these conditions, complete removal of NO3- (1.1 h-1 speed), 20 ± 2.7% of organic matter removal (366.5 ± 3.5 mg COD L-1)> 90% ethanol removal were obtained. Based on the mass sequencing of the 16 S rRNA gene via the Illumina platform, bacteria related to the degradation of recalcitrant compounds were identified, such as Pseudomonas (1.5%), Zoogloea (1.73%) and Rhodanobacter (1.63%). The enzymes involved in denitrification were also inferred, such as nitrate transporters and several reductases involved in the conversion of intermediates. Although ibuprofen removal occurred in the absence of ethanol (16.5%) and nitrate (15.2%), the optimal removal range (97.5%) as well as the selection of bacteria possibly involved in its degradation pathways was obtained with 110.6 mg EtOH L-1 and 95.9 mg NO3- L-1,

achieving removal approximately 5.9 times higher when compared to the assays without ethanol and nitrate.

- **Keywords:** Recalcitrant compounds; Co-substrate; Denitrification; Rotational central compound design

Aroosh Shabbir, Hamid Mukhtar, Muhammad Waseem Mumtaz, Umer Rashid, Ghulam Abbas, Bryan R. Moser, Ali Alsalme, Tooba Touqeer, Chawalit Ngamcharussrivichai. *Lewatit-immobilized lipase from Bacillus pumilus as a new catalyst for biodiesel production from tallow: Response surface optimization, fuel properties and exhaust emissions*. Pages 286-296.

Biodiesel is currently regarded as a sustainable and renewable alternative to depleting fossil fuels such as petro-diesel. Biodiesel production on a large scale could have a positive impact on the energy sector and the environment by lowering greenhouse gas emissions. Disadvantages of biodiesel include utilization of high-cost edible oils for production of biofuels, generation of wastewater and inability to recycle catalysts after alkaline-catalyzed methanolysis. The objectives of the current study were to utilize low-cost, inedible tallow to produce biodiesel from Lewatit-immobilized lipase produced from Bacillus pumilus and to measure the fuel properties and exhaust emissions of the resulting fatty acid methyl esters. Response surface methodology was used to optimize reaction conditions and alkaline (potassium hydroxide; KOH) catalysis was performed for comparison. A conversion of 96% was achieved by two step chemical-mediated transesterification, whereas conversion was 67% for the single step lipase-mediated method. Acid pre-treatment was needed in the case of KOH-catalyzed transesterification to reduce the acid value of tallow from 17.6 to 1.3 mg KOH/g, whereas the Lewatit-immobilized lipase was able to efficiently catalyse both transesterification of glycerides and esterification of free fatty acids. To the best of our knowledge, the lipase from B. pumilus has not yet been studied for biodiesel production from tallow. Fuel properties of the resulting optimized biodiesel were within the limits prescribed in ASTM D6751 and EN 14214. In addition, exhaust emissions studies revealed reduced CO and PM relative to petro-diesel. In both cases, reductions were greater as the percentage of biodiesel increased in blends with petro-diesel. However, NOx emissions were elevated versus petrodiesel in blends that contained 50% or more of biodiesel. This research reveals new ways for utilization of waste animal fats for biodiesel production as well as a new efficient lipase source that yields more products and provides environmental and economic security.

- **Keywords:** Tallow; Biodiesel; Transesterification; Response surface methodology; Bacillus pumilus; Lewatit-immobilized lipase; Fatty acid methyl esters

Basir Maleki, S. Siamak Ashraf Talesh. *Cold flow properties and CI engine parameters synchronic improvement of biodiesel/diesel/ C3 and C4 alcohol blends: Mixture design approach*. Pages 310-326.

The rising demands of fuel and petrochemical fuels that have harmful gas emissions are encouraging researchers to develop green fuels, especially biodiesel. Whereas the substantial restriction for utilizing biodiesel as a replacement fuel is poor cold flow properties. This research aimed to consider the synchronic improvement of canola biodiesel-diesel-alcohols mixture with low-temperature performance and diesel engine parameters. The simplex lattice mixture design method was applied to optimize, statistically analyze, and design fuel-blend experiments. The best-fitted values via the models were verified employing analysis of variance. Optimum conditions for the cold flow properties of the ternary fuel blends were achieved at biodiesel (19.3), diesel (41.7), and alcohol (39) v/v.%, named as B19.3-Bu39. At the optimum, the best cold flow

properties had a pour point and cloud point of − 22.67 and − 16.37 0C. Engine performance results revealed that increment of higher alcohols in fuel blend enhanced brake specific fuel consumption (6.22%) and exhaust gas temperature (16.25%), while the brake thermal efficiency (4.03%) diminished. At the maximum loading, emission reductions of 13% and 49% of carbon monoxide, and 20.3% and 30.5% of unburned hydrocarbon were achieved for B19.3 and B100 (100% biodiesel). Oxidative stability of the optimum fuel blend was 10.32 h, which is satisfactory according to EN14214 standard. Results implied that the B19.3-Bu39 fuel has superior lubrication, lower emission, wear, and friction as compared to pure diesel. It can be concluded that the incorporation of higher alcohols presents a novel prospect for the simultaneous improvement of fuel cold flow properties and CI engine operability parameters.

- **Keywords:** Biodiesel; Fuel blend; Higher alcohols; Cold flow properties; Engine parameters; Simplex lattice mixture design method

Zhenyu Deng, Te Han, Zhonghai Cheng, Jiajia Jiang, Fajie Duan. *Fault detection of petrochemical process based on space-time compressed matrix and Naive Bayes*. Pages 327-340.

Due to the high available and reliable requirements of petrochemical processes, it is critical to develop real-time fault detection approaches with high performance. Some machine learning approaches have shown good results but the learning process is too complicated to meet the requirements of online application, such as plenty of samples or the laborious hyper-parameter optimization is needed. In this paper, a fault detection approach based on space-time compressed matrix (STCM) and Naive Bayes (NB) is proposed to realize the fast learning and prediction. First, the slowly varying features which reflect the inherent dynamic information of petrochemical processes are extracted by slow feature analysis. Second, the accumulative importance of slow features and the reconstructive advantage of slow feature under-sampling are proposed to achieve the space-time compression of data matrix. Finally, the STCM is employed to establish the NB model, which can significantly reduce the learning complexity while ensuring classification performance. Experiments on the Tennessee Eastman benchmark show that the proposed approach reduces the sample-size and feature-size by 75% and 92% respectively. Both the average classification accuracy and F1 score on 21 faults exceed 84%, achieving the state-of-the-art results among the comparative approaches.

- **Keywords:** Fault detection; Petrochemical process; Slow feature analysis; Space-time compressed matrix; Machine learning

Jishuo Li, Xiwen Yao, Shoukun Chen, Kaili Xu, Bingjie Fan, Dexin Yang, Liyan Geng, Haiming Qiao. *Investigation on the co-pyrolysis of agricultural waste and high-density polyethylene using TG-FTIR and artificial neural network modelling*. Pages 341-353.

To realize utilization of agricultural and plastic waste to alleviate environmental pollution, the individual pyrolysis and co-pyrolysis characteristics of kidney beans stalk (KS) and high-density polyethylene (HDPE) were investigated. Thermogravimetry coupled with Fourier transform infrared spectroscopy (TG-FTIR) was used to investigate the pyrolysis behaviour, synergistic effect, kinetics and gaseous product evolution of different samples. In addition, an artificial neural network (ANN) model was established to predict the mass change with temperature during sample pyrolysis or co-pyrolysis. The results showed that the decomposition of HDPE was easier than that of KS, and synergistic and inhibitive effects occurred during co-pyrolysis. The synergistic or inhibitive effect was most significant from 470 to 510 ℃. The FTIR analysis results showed that gaseous products of KS pyrolysis were mainly oxygen-containing compounds including CO2, CO, ketones, aldehydes, esters, etc., while those of HDPE pyrolysis were mainly hydrocarbons

including alkanes, alkenes, aromatic rings, etc. The co-pyrolysis of samples with different proportions promoted or inhibited the production of some gaseous products to different degrees. Moreover, the activation energy of the two stages during co-pyrolysis was lower than that of the pure sample. The established ANN model can effectively predict the mass loss of a sample with temperature.

- **Keywords:** Agricultural waste; HDPE; TG-FTIR; Synergistic effect; ANN

Monika Niemczyk, Parvin Berenjkar, Richard Sparling, Stan Lozecznik, Qiuyan Yuan. *Optimized design of a compost layer in a landfill biocover for CH4 oxidation*. Pages 354-361.

In this study, the mixture of two compost materials, including Yard Waste and Leaf Compost (YWLC) and Biosolids Compost (BSC) was optimized for methane (CH4) oxidation to be suitable for a field-scale landfill biocover. Laboratory column tests were conducted with CH4 and carbon dioxide (CO2) flowing through the column at 50:50 v:v to assess the CH4 oxidation in the vertical profile of the compost. The variation in CO2:CH4 ratio, indicating methanotrophic activity, was assessed during three column trials considering two different mixing ratios of 1:1 and 1:4 YWLC:BSC, moisture contents (MC) of 60%, 35%, and 40% ww, and the addition of a methanotroph-enriched compost extract. It was found that the main restricting factors for effective CH4 oxidation were high MC, Exopolymeric Substance (EPS) formation, and fine texture of the materials that limited oxygen (O2) diffusion into the biocover. Based on CH4 mass balance in the columns, the highest CH4 oxidation efficiency of 40% was observed in the column trial with the 1:4 mixing ratio of composts at a MC of 40% ww, with CH4 being oxidized throughout the entire height of the column. It can be concluded that this optimized design for YWLC and BSC mixture, removing a significant portion of the CH4 flowing through the landfill biocover, had the potential to be used in the real field conditions.

- **Keywords:** Methanotrophs; Landfill biocover; Compost; Column test; Permeability

P. Márquez, J.A. Siles, M.C. Gutiérrez, J. Alhama, C. Michán, M.A. Martín. *A comparative study between the biofiltration for air contaminated with limonene or butyric acid using a combination of olfactometric, physico-chemical and genomic approaches*. Pages 362-375.

A multidisciplinary analysis based on physico-chemical, olfactometric and microbiological perspectives was performed to compare the biofiltration of air contaminated with limonene or butyric acid. Two biofilters were subjected to butyric acid gaseous streams: one was filled with wood chips and sewage sludge compost (BF B-1) and the other with wood chips only (BF B-2). Similarly, two other biofilters were subjected to a gaseous stream containing limonene, with the same beds (BF L-1 and BF L-2, respectively). Although the biofilters fed with butyric acid received higher odor loads (280–3280 ouE/m2·s for BF B-1 and 135–1460 ouE/m2·s for BF B-2) than the biofilters treating limonene (30–170 ouE/m2·s for BF L-1 and 15–130 ouE/m2·s for BF L-2), the first systems achieved odor removal efficiencies greater than 90% during most of the biofiltration time, whereas in the limonene biofilters, these efficiencies never exceeded 70%. Regarding the packed beds, genomic analysis of the microbial communities showed a wider distribution of phyla (Proteobacteria, Firmicutes, Bacteroidetes, and Actinobacteria) in compost-wood biofilters than in wood chips systems where Proteobacteria was clearly predominant. This study reveals the importance of considering both the nature of the biofiltered compounds and the packed bed composition in biofiltration operations.

- **Keywords:** Biofiltration; Butyric acid; Packing material; Genomic analysis; Limonene; Odor removal

Gaofeng Zhou, Yongsheng Fu, Runyu Zhou, Li Zhang, Linyue Zhang, Jiewen Deng, Yiqing Liu. *Efficient degradation of organic contaminants by magnetic cobalt ferrite combined with peracetic acid*. Pages 376-384.

In this study, a novel heterogeneous peracetic acid (PAA)-based advanced oxidation process (AOP), viz. cobalt ferrite combined with PAA (CoFe2O4/PAA), was used to degrade organic contaminants. The best pH for rhodamine B (RhB) degradation in CoFe2O4/PAA system was at 7, and approximately 95% RhB could be removed within 10 min at this pH. Radical scavenging experiments indicated that organic radicals (i.e., CH3COO• and CH3COOO•) were the dominant reactive species for RhB degradation. The X-ray photoelectron spectroscopy (XPS) analysis for the fresh and used catalysts suggested that the catalytic reaction mainly occurred on the surface of the catalyst. Increasing PAA dosage and CoFe2O4 dosage could enhance the removal of RhB, while excess CoFe2O4 dosage inhibited its degradation probably due to the clumping effect of magnetic nanoparticles. Five degradation products of RhB by CoFe2O4/PAA were identified and two degradation pathways of RhB were subsequently proposed, including bond cleavage and hydroxylation. CoFe2O4 exhibited an excellent stability and reusability, and the removal rate of RhB could maintain at 92.4% after four cycles. Several kinds of organic contaminants were selected to evaluate the applicability of CoFe2O4/PAA system, and the results suggested that CoFe2O4/PAA system exhibited a selectivity for different contaminants.

- **Keywords:** Organic radicals; Advanced oxidation process; Heterogeneous catalysis; Rhodamine B; Degradation products

Gang Fu, Lei Ni, Dan Wei, Juncheng Jiang, Zhiquan Chen, Yong Pan. *Scale-up and safety of toluene nitration in a meso-scale flow reactor*. Pages 385-396.

In this study, toluene nitration was scaled up in a meso-scale flow reactor and safety was considered. The exothermic characteristic was demonstrated in a batch calorimeter. Parallel flow was observed in the flow channel and numerical simulation was carried out to show the hydrodynamics. Mass transfer coefficient of the reactor mixer was determined. The effects of flow rates, temperatures and molar ratios on toluene nitration in the flow reactor were analyzed. The conversion of toluene increased from 26% to 86% with the increase of flow rates while the impacts of temperatures and molar ratios were comparatively small. A productivity of 2572 kg/a could be achieved by this meso-scale flow reactor but the highest overtemperature inside the channel was more than 21.3 ◦C. A comparison between performances of the batch calorimeter and the flow reactor was also presented. The finding of this study can serve as a reference to design inherently safer meso-scale flow reactors for kinetically fast and highly-exothermic reactions.

- **Keywords:** Microreactor; Scale-up; Two-phase flow; Mass transfer; Numerical simulation

Xin Huo, Qiang Lu, Jian Wang. *Liaw-UNIFAC flash point model for alcohols-kerosene/diesel fuel blends using average fuel structure*. Pages 400-410.

Alcohol has already been widely used as an alternative fuel to blend with petroleum-based fuels. Accurate knowledge of flash points and their reliable prediction methods is essential in hazard identification, fire hazard reduction, process inherently safer design, and the risk management of alcohol-based fuels. This work presents a model to predict the flash point for alcohol + petroleum-based fuel blends based on the Liaw model incorporated with the original UNIFAC model. The flash point prediction model was modified by two steps: 1. applying a single vapor-temperature relationship for the

petroleum-based fuel; 2. obtaining the activity coefficients by UNIFAC model using an average fuel structure for the petroleum-based fuel. The proposed model was verified experimentally for five fuel blends of alcohol + kerosene (alcohol being n-butanol, n-hexanol, and n-octanol) and alcohol + diesel (alcohol being n-butanol and n-hexanol). The flash point prediction procedure for alcohol + petroleum-based fuel blends was reduced to that of a binary mixture. The deviations between the predicted values and experimental data were mostly within 2 °C for the five fuel blends.

- **Keywords:** Flash point; Kerosene; Alcohol; UNIFAC model; Group structure

Bächler P., Löschner V., Meyer J., Dittler A. *Process integrated monitoring of spatially resolved particle emissions of a baghouse filter using a network of low-cost PM-sensors*. Pages 411-423.

In industrial applications of baghouse filters, emission sources other than direct penetration contribute greatly to the overall outlet dust emission. Spatio-temporal process monitoring could enable the detection of local particle emission hotspots and facilitate maintenance procedures by offering new insights regarding the emission behavior of baghouse filters. This publication shows the spatial emission behavior measured by low-cost sensors in a small scale baghouse filter with nine filter bags. After initial cleaning cycles, which cause clogging of the seams and a decrease of the particle emission level, the emission behavior corresponds to ideal filter operation. However, seemingly random continuous particle emissions are temporarily measured at individual filter bags within the baghouse. Via spatial monitoring and comparison with the total dust emission of the process, measured by a state-of-the-art precision laboratory optical particle counter, these events can be allocated to a corresponding filter bag, which serves as the source of temporary increase in dust emission. An increase in tank pressure shows a rise of the intensity and frequency of temporarily occurring continuous emissions. This behavior can be directly linked to a release of particles from previously clogged seams, thus enabling renewed particle penetration through the stitching holes of the seams.

- **Keywords:** Baghouse filter; Surface filtration; Low-cost PM-sensor; Process monitoring; Leak detection; Dust separation; Emission control

Yunfeng Xu, Chuyin Liu, Yangwei Qu, Ying Ding, Jia Zhang. *Modified pineapple peel extract coupled with electrokinetic techniques for remediation of chromium-contaminated soil*. Pages 424-433.

Remediation of chromium (Cr)-contaminated soil is a hot topic in environmental science and technology. In this field, one important issue is to develop a low-cost and effective electrolyte. This work investigated efficient remediation of Cr-contaminated soils by electrokinetic using pineapple-peel extract (PPE) as electrolyte. The main components of PPE were sugar and citric acid. The effects of these two components were investigated on remediation efficiency. The changes of soil properties, including pH, conductivity, electroosmotic flow, and Cr residue, were detailedly analyzed during electrokinetic remediation. After modification by H2O2, total sugar and organic acid contents in PPE changed from 64.5% and 0.115–42.5% and 0.304%, respectively. These changes further improved the Cr remediation. The highest average removal was 82.75% when 30% of H2O2 was used to modify PPE electrolyte. The main result of this work is in favor of developing and applying green electrolyte in electrokinetic technology. At the same time, pineapple residual is effectively recycled, which is devoted to green development.

- **Keywords:** Chromium-contaminated soil; Electrokinetic remediation; Electrolyte; Pineapple-peel extract; Modification

Huixing Meng, Xu An, Jinduo Xing. *A data-driven Bayesian network model integrating physical knowledge for prioritization of risk influencing factors*. Pages 434-449.

The coupling of multiple factors stemming from propagation effects and interdependency relationships among risks is prone to generate major accidents. It is of necessity to develop a feasible model with limited cases, which can generate reliable causal relationship evolution. To prioritize risk-influencing factors (RIFs) and investigate their relationships, we proposed a data-driven Bayesian Network (BN) model integrating physical information for risk analysis. Based on collected data, we combined prior knowledge with structure learning and parameter learning to obtain a BN model. In structure learning, we compared three structure learning algorithms including Bayesian search (BS), greedy thick thinning (GTT), and PC algorithm to obtain a robust directed acyclic graph (DAG). In parameter learning, we selected the expectation maximization (EM) algorithm to quantify the dependence and determine the probability distribution of node variables. This study provides a method to capture crucial factors and their interdependent relationships. To illustrate the applicability of the model, we developed a data-driven BN by taking the blowout accident as the case study. Eventually, we introduced vulnerability and resilience metrics for prioritizing risks through network propagation to conduct emergency plans and mitigation strategies.

- **Keywords:** Data-driven; Bayesian network; Risk-influencing factor; Prioritizing risks

Abdolmotaleb Seid-Mohammadi, Ghorban Asgari, Mohammad Rafiee, Mohammad Taghi Samadi, Fatemeh Nouri, Meghdad Pirsaheb, Fateme Asadi. *Fate and inhibition of Bis (2-Ethylhexyl) phthalate in biophysical reactors for treating real landfill leachate*. Pages 450-464.

In this study, the performance of combined Non-Thermal Plasma (as a pre-treatment) and granular sludge sequencing batch reactor (as a post-treatment) was evaluated for decontamination of real landfill leachate containing Bis (2-Ethylhexyl) phthalate. Special emphasis was placed on the biodegradability of leachate due to its high chemical stability and generation of intermediate species. A plasma reactor with a useful volume of 0.5 L, quartz material was utilized by this study for the pre-treatment process. The biological treatment efficiency was investigated using three granular sludge sequencing batch reactors, each containing 1.2 L with different apparatuses. The Hamadan landfill leachate sample was diluted with synthetic wastewater at 20%, 50%, and 100% v/v ratios. The applied influent Bis (2-Ethylhexyl) phthalate concentrations were 2, 4, 6, 8, 10, 15, and 20 mg/l. Organic loading rate in terms of COD and Bis (2-Ethylhexyl) phthalate concentrations, as well as reactor hydraulic retention time, were worked out to assess the processes performance (COD, nitrogen, phosphorus, and Bis (2-Ethylhexyl) phthalate removal efficiencies). Total Organic Carbon and 5-day Biochemical Oxygen Demand were also measured at the influent and effluent of the NTP reactor over a range of retention time (5, 10, 15, 20, 30, 45, and 60 min) to determine the degree of biodegradability enhancement. Cell protein concentration was also measured using a nanotherape device to assess the effect of DEHP inhibitor on bacterial growth. The main results arrived at from the overall assessment of the processes are that the BOD5/COD ratio of Non-Thermal Plasma reactor effluent at all leachate dilution, i.e., 20%, 50%, and 100% (v/v ratios) considerably increased, reaching 1.09 as compared to 0.33 in the raw influent. The findings indicated that the longer hydraulic retention time affected the granular sludge sequencing batch reactor efficiency. Further, cell protein concentration decreased by increasing the leachate contribution of inlet COD and increased Bis (2-Ethylhexyl) phthalate. It is concluded that Non-Thermal Plasma, as a highly competitive waste treatment technology coupled with aerobic granular sludge, could be considered for the

biodegradation of landfill leachate containing chemically stable and recalcitrant organics not treatable by conventional techniques.

- **Keywords:** Leachate; Non-thermal plasma; Aerobic granular sludge

Maryam Yavari-Bafghi, Mahmoud Shavandi, Seyed Mohammad Mehdi Dastgheib, Mohammad Ali Amoozegar. *Simultaneous application of CaO2 nanoparticles and microbial consortium in Small Bioreactor Chambers (SBCs) for phenol removal from groundwater*. Pages 465-477.

Phenols are toxic products derived from a wide range of industrial activities and the entry of these contaminants into the environment is seriously hazardous for both human and aquatic ecosystems. This study presents the use of a phenol-degrading consortium surrounded in an innovative "Small Bioreactor Chambers" (SBCs) along with biostimulation for phenol bioremediation from contaminated groundwater. To investigate the effect of biostimulation, synthesized-calcium peroxide (CaO2) nanoparticles were applied. The phenol-degrading consortium, was successfully isolated from a water well located in Iran. The highest growth rate and phenol degradation of the ph100-consortium were observed at 15 °C and pH 7.5 in the presence of 500 mg·L-1 of powdered CaO2 and 100 mg·L-1 of phenol as a sole source of carbon. Next-generation sequencing (NGS) analysis of the consortium revealed that Proteobacteria and Bacteroidetes with 75.3% and 16.2% relative abundance were the dominant phyla in the ph100-consortium, respectively. Experimental results indicated that 100% of the contaminant (100 mg·L-1) was successfully removed from groundwater using encapsulated CaO2 within 60 days with the negligible negative impacts on the microbial population. Furthermore, the highest biodegradation percentage were achieved during incubation of SBCs in a medium supplemented with 500 mg·L-1 CaO2 powder in 25th days of experiment. These results provide certain evidence for a successful simultaneous application of biostimulation and bioaugmentation processes through SBCs for contaminated water treatment.

- **Keywords:** Bioremediation; CaO2; Small Bioreactor Chambers (SBCs); Groundwater; Phenol

Ashwin Jacob, B. Ashok, Kaisan Muhammad Usman. *Production of Chlorella pyrenoidosa biodiesel by heterotrophic pathway to improve CI engine output characteristics using statistical approaches*. Pages 478-490.

An alarming rise in greenhouse gases originating from on-road vehicles and the rapid depletion of cultivable land for fuel feedstocks has led researchers to explore alternative means of biofuel production. In this context, the current study explores the heterotrophic cultivation of Chlorella pyrenoidosa microalgae by scaling-up using various combinations of stir-tank bioreactors for the sustainable synthesis of low-density biodiesel. Furthermore, statistical tools are employed to develop prediction models to incorporate 20% (vol/vol) of the low-density biodiesel with diesel fuel (CP20) to obtain optimal experimental outputs. From the study, it was found that the percentage dry cell weight of samples acquired from 100 L, 200 L and 300 L stir tank bioreactors achieved 44.1%, 46.7% and 41% of lipid content and biomass concentrations of 5.15 g/L, 4.24 g/L and 4.36 g/L on up-scaling. At an optimal reaction temperature and time of 37 °C and 12 h, the highest biodiesel conversion rate of 98% was achieved during enzymatic transesterification. The prediction engine models reveals that at the finest engine input parameter combinations, 0.74% improvement in brake thermal efficiency and a 50% drop in smoke emissions are achieved using the low-density CP20 blend. Also, superior combustion characteristics are delivered on operation as a trade-off for NOX emissions.

- **Keywords:** Heterotrophic cultivation; Low-density biodiesel; Microalgae feedstock; Emission control; Prediction models; Design of experiments

Kakeru Shibue, Yuta Sugiyama, Akiko Matsuo. *Numerical study of the effect on blast-wave mitigation of the quasi-steady drag force from a layer of water droplets sprayed into a confined geometry*. Pages 491-501.

The blast-mitigation effect produced by water droplets sprayed into a confined geometry was studied. When a one-dimensional blast wave interacts with a layer of water droplets, blast mitigation occurs that can be expected to reduce the damage from an accidental explosion. Focus was on the blast-mitigation effect produced by the quasi-steady drag force between the shocked air and the stationary water droplets. Momentum transfer due to the drag mitigated the blast wave, and the maximum blast-wave mitigation occurred just behind the layer of droplets. The study parameters (the volume fraction of water droplets, the location and length of the region with sprayed water droplets, and the mass of the high explosive) demonstrated that higher momentum loss from the air resulted in greater mitigation. The momentum loss was evaluated using the volume fraction and length of the layer of water droplets and the quasi-steady drag force when the shock wave reached the layer. Relationships were formulated between the initial conditions, the momentum loss, and the blast-mitigation effect, which made it possible to evaluate quantitatively the mitigation effect on the blast wave caused by the water droplets.

- **Keywords:** Blast mitigation; Water droplets; Confined geometry; Quasi-steady drag; Momentum loss

Elmehdi Moumen, Loubna Bazzi, Samir El Hankari. *Aluminum-fumarate based MOF: A promising environmentally friendly adsorbent for the removal of phosphate*. Pages 502-512.

The removal of excessive phosphate from water is very important to avoid eutrophication. For this purpose, metal-organic frameworks (MOFs) have recently attracted great attention in phosphate adsorption due to their outstanding physicochemical features. However, most of the used MOFs in the adsorption of phosphate are based on those synthesized from organic ligands derived from petroleum sources such as tricarboxylic (BTC) and dicarboxylic acid (BDC), which can negatively impact the environment. Consequently, using stable MOF synthesized from an eco-friendly ligand is highly desired. In this work, Aluminum based fumarate MOF (Al-Fum) was used in the adsorption of phosphate from water and subsequently compared with other Al-MOF derived dicarboxylic acid (Al-BDC) and tricarboxylic acid (Al-BTC). The phosphate adsorption performance of the different synthesized Al-MOFs was evaluated with the help of different batch experiments related to the effect of adsorbent/adsorbate concentrations, the contact time, the pH and the temperature. Interestingly, Al-Fum displayed the highest adsorption capacity (67,62 mg P/g) compared to Al-BDC (47,58 mg P/g) and Al-BTC (23,17 mg P/g) at RT (22,2 °C). The regeneration of Al-Fum was tested for several cycles showing continuous adsorption capacity and stability. This work opens a new avenue toward the development and use of more environmentally friendly and reused MOFs for the removal of phosphate from water.

- **Keywords:** Adsorption; Aluminum fumarate; Environmentally friendly MOF; Metal-organic frameworks; Phosphate removal

Ján Janošovský, Igor Rosa, Gregor Vincent, Branislav Šulgan, Miroslav Variny, Zuzana Labovská, Juraj Labovský, Ľudovít Jelemenský. *Methodology for selection of inherently safer process design alternatives based on safety indices*. Pages 513-526.

Safety is a key part of any modern production process and as such is reflected in legislation and work regulations. Decision-making concept based on inherently safer design principles is introduced in this paper. Two case studies representing typical modern chemical processes are studied with the emphasis on their inherent safety level. First case study is a novel process to convert refinery waste into valuable products – production of ammonium thiosulphate. As a second case study, production of ethyl acetate by esterification was selected due to its potential for process intensification through reactive distillation. For each case study, two design alternatives are proposed. Utilising process data, the design alternatives are evaluated using five safety indices and compared to each other to identify the inherently safer one considering fire and explosion hazards as well as toxicity level. Results show that different sensitivity of index methods can lead to different outcomes of hazard potential identification. For the second case study, results of each method were in agreement. However, reverse order of design alternatives was obtained in the analysis of the first case study. As a part of this article, novel processing technique employing geometry of polygons to assess hazard distribution and inherent safety level of different process routes has been introduced and employed. Obtained results suggest possible implementation of the proposed approach to robust multi-criteria decision analysis as a safety assessment criterion.

- **Keywords:** Inherently safer design; Aspen Plus; Safety index; Decision-making

Lingqiang Yan, Jinlong Li, Qing Ye, Xue Jian, Xinhao Li, Licheng Xie, Jianyu Zhang. *Sustainable wastewater treatment via extractive distillation process with ionic liquid as entrainer for the separation of ethyl acetate/isopropanol/water*. Pages 527-540.

To recycle isopropanol and ethyl acetate from wastewater by extractive distillation, 1-butyl-3-methylimidazolium acetate ([BMIM][OAc]) is considered to be an appropriate entrainer by comparing with ethylene glycol on VLE diagram and σ-Profiles, respectively. Then, the extractive distillation processes with [BMIM][OAc] as entrainer are proposed. Since the degradation temperature of [BMIM][OAc] requires the entrainer recovery section of processes to operate under high vacuum, one-stage evaporator and one stripping column configuration is determined to recycle entrainer [BMIM][OAc]. After optimizing the IL processes, the heat integration technology is applied to the optimized processes. Compared conventional extractive distillation process with EG as entrainer, the heat integration assisted IL process with appropriate entrainer recovery configuration which uses IPA as stripping agent can reduce 24.76% of TAC, 45.64% of energy consumption and 45.52% of gas emission.

- **Keywords:** Extractive distillation; Ionic liquid; Separation effect; Entrainer recovery; Heat integration

Xiaofan Li, Guochun Lv, Ning Wang, Xiaomin Sun, Xiang Li, Mei Li. *Theoretical insights into the transformation mechanism and eco-toxicity effects of 5-Fluorouracil by O3 and OH in waters*. Pages 541-550.

The existences of non-biodegradable 5-Fluorouracil (5-FU) in aquatic systems and its potential toxic effects on aquatic organisms have caused widespread concern. In this work, two typical oxidants (O3 and ·OH) were selected to investigate the mechanism, kinetics, and the potential eco-toxicology assessment of 5-FU using computational chemistry methods. Results show that 5-FU can be degraded rapidly by O3 and ·OH, which subsequently undergoes ring-opening, decomposition, defluorination, and hydroxylation steps. The rate constants of initiation reactions are suppressed as the temperature increases. The half-lives of 5-FU determined by O3 and ·OH are on the order of seconds in the advanced oxidation processes (AOPs) system. Fifteen structures of transformation products were identified by theoretical calculation, including five

experimental products. The toxicity assessment results show that the acute and chronic toxicities of the degradation process to aquatic organisms gradually decreased, but the developmental toxicity and mutagenicity of several products on human still exist. In addition, the main products have been found to decompose into some small molecules (NO, Formic acid, Acetic acid, etc.). This result could help to reveal the transformation behaviors and risk assessment of 5-FU in aquatic environments, and further design the experimental and industrial infrastructure.

- **Keywords:** 5-Fluorouracil; Ozone; OH radical; Transformation mechanism; Kinetics analysis; Eco-toxicity assessment

Xingwei Zhen, Jan Erik Vinnem, Yue Han, Changyi Peng, Yi Huang. *Development and prospects of major accident indicators in the offshore petroleum sector*. Pages 551-562.

In recent years, several major accidents, such as the US Macondo well blowout in 2010, Chinese Bohai Bay oil spills in 2011, Brazilian FPSO Cidade de São Mateus gas explosion in 2015 and Chinese Bohai oil field blowout & fire accident in 2021, have provoked a high awareness that an essential distinction exists between the major accident management and the occupational accident management in the offshore petroleum sector. Further, the urgent need for defining effective major accident indicators is confirmed for the purpose of identifying early warning signals before the major offshore accident occurs. Regrettably, to this day, the offshore petroleum sector has not reached a consensus on the theoretical foundation for the development of effective major accident indicators. This article presents a focused review on the extensive work of the development of major accident indicators in the offshore petroleum sector, including terminologies, assessment criteria for good indicators, development approaches, as well as an overview of current major accident indicators. Following the close scrutiny of this focused review, the strengths and weaknesses of different development approaches are compared. The progress, challenges, suitability and validity of the development of major accident indicators are discussed. On the basis of these insights, future works are suggested to develop effective major accident indicators to better engage on the emerging and complex challenges in preventing major offshore accidents.

- **Keywords:** Major accident; Indicators; Criteria; Barriers; Performance; Offshore

Xiaoxiao Liu, Shuiying Zhong, Shan Li, Mian Yang. *Evaluating the impact of central environmental protection inspection on air pollution: An empirical research in China*. Pages 563-572.

Based on the panel data of various daily air pollution indicators of 288 prefecture-level cities in China from January 1, 2015 to December 31, 2018, this paper takes the first round of central environmental protection inspection (CEPI) as a quasi-natural experiment, and empirically analyzes its impact on urban air pollution by using multi-period difference-in-difference (DID) method. The results show that: (1) the first round of five batches of environmental inspection and two batches of "looking back" have significantly reduced the concentration of seven pollutants; (2) The first five batches of environmental inspection have a stronger impact on reducing air pollution than "looking back"; Moreover, in the short term after the inspection, it still has a significant reduction effect on air pollution; (3) The impact of central environmental protection inspection on air pollution shows strong heterogeneity in different batches of inspections, urban scale and economic development level, as well as the air quality level of cities before the inspection. The research results of this paper provide corresponding policy recommendations and decision-making basis for the Chinese central government to further deepen the reform of environmental protection supervision mechanism and promote the emissions of multiple pollutants mitigation.

- **Keywords:** Central environmental protection inspection; Air pollution; City-level panel data; Multi-period DID model

Zhengjun Gu, Xinmei Wang, Pu Huang, Yu Huang, Xuan He, Xinzheng Wei, Jiahe Yue, Juncheng Jiang, Chuanwen Zhao. *Experimental and kinetics investigations of low-concentration CO2 adsorption on several amine-functionalized adsorbents*. Pages 573-583.

The rapid cleanup of endogenous CO2 has become a necessity in environmental control and life support systems (ECLSSs), to ensure crew safety and long-term task execution. The extensively used non-regenerable LiOH and soda lime adsorbents, although exhibit high CO2 storage capacities and fast kinetics, can hardly fulfill the demands of reduced launch weight and storage volume in the space- and load-limited ECLSSs. New CO2 adsorbents with desirable attributes including high CO2 uptakes, good selectivity, facile regeneration, fast adsorption and desorption kinetics, and good multicycle stability are urgently needed. We developed amine-functionalized adsorbents by loading tetraethylenepentamine (TEPA) on mesoporous supports of activated carbon (AC), aluminum oxide (AO) and silica gel (SG). The adsorbents were characterized by N2 adsorption-desorption, thermogravimetric analysis (TGA), Fourier transform infrared spectroscopy (FT-IR), and scanning electron microscope (SEM) to study their microstructural properties. CO2 adsorption capacities and kinetic performance of the adsorbents with different supports and various amine loadings (10–50 wt%) were evaluated in 2%CO2 at 20 °C. The effects of support and amine loading on the structure-performance relationships of the adsorbents were demonstrated. The TEPA-SG-20 adsorbent (20 wt% TEPA loaded on silica gel support) exhibits the highest CO2 adsorption capacity of 1.90 mmol CO2/g and the maximum amine efficiency of 0.48 mmol CO2/mmol N. TEPA-SG-20 also exhibits fast CO2 adsorption kinetics, and the Avrami fractional order kinetic model provides a satisfactory correlation of the experimental CO2 uptakes. Furthermore, the TEPA-SG-20 adsorbent can be efficiently regenerated at 110 °C with a great regeneration efficacy of 97%. The desired adsorbent also exhibits good working stability with a low loss-in-capacity of 4.32% in 10 consecutive cycles. The good CO2 adsorption performance of TEPA-SG-20 is associated with the excellent microstructural properties such as high surface area, great pore volume and uniform dispersion of amine species. Overall, the desired TEPA-SG-20 adsorbent shows promise for low-concentration CO2 removal in ECLSSs.

- **Keywords:** Amine-functionalized adsorbents; Structure-performance relationships; Support effect; Amine loading; CO2 adsorption capacity; Kinetic performance

Zhen Qin, Zaoxiao Zhang, Xiaoqian Ma. *Effects of sewage sludge blending on techno-economic performance of Integrated Gasification Combined Cycle (IGCC) system*. Pages 584-593.

Municipal sewage sludge (SS) can be used as an alternative carbon-neutral feedstock for energy utilization owing to its considerable higher heating value compared with lignite coal. It is potential to efficiently co-utilize SS by coal-sludge-slurry gasification technology avoiding the energy consumption for SS drying process. In this study the effects of SS blending on the techno-economic performance of Integrated Gasification Combined Cycle (IGCC) systems based on different kinds of gasification technology and coal are analyzed. The results show that the overall energy efficiency of the system based on dry gasifier is more sensitively affected by the blending of SS than the one based on wet gasification due to the energy consumption during drying process. For wet gasification technology, the overall energy efficiency for coal A first increases from 45.17% to 45.26% and then reduces to 44.77% with the SS mix ratio, while the overall energy efficiency for coal C declines from 38.58% to 38.03%. The results indicate the

overall energy efficiency has positive correlation with the cold gas efficiency instead of ash fusion temperature and the effects of SS addition on the overall energy efficiency can be qualitatively estimated by analyzing the cold gas efficiency. In most cases the blending of SS in IGCC systems benefits the economic performance and the net present value of the system based on wet gasification and coal A could be increased by 88% due to the increasing power output and the SS treatment subsidy.

- **Keywords:** Sewage sludge; IGCC; Coal sludge slurry; Dry gasification; Techno-economic analysis

Shibani, Fatemeh Salehi, Til Baalisampang, Rouzbeh Abbassi. *Numerical modeling towards the safety assessment of multiple hydrogen fires in confined areas*. Pages 594-609.

Hydrogen fuel cell vehicles (FCVs) have been considered an option for the future zero-emission transport sector. However, there are some safety concerns about FCVs in restricted environments. Risk analysis of possible fire scenarios is an efficient approach to identifying, evaluating, and mitigating the risk from hydrogen fire accidents. Computational fluid dynamics (CFD) simulations were conducted for a 102 m long tunnel to analyse the influence of multiple hydrogen fires having different heat release rates (HRR). The developed model was first validated against published data. A detailed computational analysis of multiple hydrogen fires was then conducted to understand the influence of HRR, leakage area, ventilation velocity, the presence of sloping, and the sealing ratio of the tunnel. In the absence of inlet velocity, the high thermal zones are closer to the tunnel ceiling at the fire's location. With increasing the inlet air velocity, the overall ceiling temperature reduces, although the high-temperature zones are pushed further downstream. Increasing the leakage area enhances the HRR, and hence the impact of the heat feedback mechanism becomes more significant since larger HRRs account for higher temperatures, strong flame interactions, and low oxygen concentrations. The results show that the higher sealing ratio of the tunnel leads to an increase in the peak ceiling temperatures. It is also observed that the presence of sloping increases the severity of fires as high-temperature zones and oxygen deficiency is observed at the higher locations of the tunnel from ground level.

- **Keywords:** Computational fluid dynamics (CFD); Safety assessment; Hydrogen fires, tunnel safety

Gang Liang, Shasha Li, Xiaodong Yu, Qingwei Bu, Han Qu, Hong Zhu, Xiaolong Yao, Anxiang Lu, Wenwen Gong. *Black carbon-mediated degradation of organic pollutants: A critical review*. Pages 610-619.

Black carbon (BC) has a large specific surface area and abundant surface functional groups, so it is traditionally regarded as an adsorbent and a metal catalyst carrier. In addition to this, it has recently been found that a variety of BCs can also be used as a metal-free catalyst to mediate the transformation and degradation of specific organic pollutants at room temperature. This paper reviews the recent findings and current developments of the mediating roles of BC in both chemical and microbial degradation of organic pollutants, including azo dyes, nitroaromatic compounds and halogenated hydrocarbons. It starts with a brief overview of the source, properties and sorption characteristics of BC and focuses on the mediating effects and mechanisms of various BCs (such as activated carbon, chars, graphite), as well as types of surface-modified carbon materials, on the transformation and degradation of organic pollutants. Moreover, it also introduces the research on engineered carbon-based nanomaterials (i.e., carbon nanotubes and graphene), which have similar physical and chemical characteristics, for reference. Finally, the application prospects of using BC as a metal-free catalyst to mediate the transformation and degradation of organic pollutants are discussed to provide a reference and expand new ideas for further research in this field.

- **Keywords:** Black carbon; Engineered carbon-based nanomaterials; Organic pollutants; Metal-free catalysts; Redox-mediator; Transformation and degradation

Fanyi Meng, Chang Li, Paul Amyotte, Yajie Bu, Chunmiao Yuan, Weidong Yan, Gang Li. *Effect of inclination angle on fire hazard of melting dust layers.* Pages 620-631.

Combustible dusts deposited on ground or surfaces present a fire hazard to process industries. It was found that flame spread on an upwardly inclined surface was significantly faster than on a horizontal surface. However, hazard during downward inclined fire spread has been underestimated for dust layers having melting capability. In this paper, the effects of melting fluidity, sample inclination angle, and layer thickness on the fire hazard of four melting dusts were investigated. For sulfur with its excellent melting fluidity, dust layer inclination at a small angle can significantly increase downward flame spread velocity (FSV). For anthraquinone having a moderate melting fluidity, upward or downward dust layer inclination significantly increased FSV. For polystyrene and magnesium having weak melting fluidity, dust layer inclination angle had relatively little effect on flame propagation. Increasing thickness of dust layers significantly enhanced the promotion effect of the inclination angle on the flow of molten material, which in turn affected FSV. As a result, melting fluidity coupled with a large inclination angle and high layer thickness would significantly enhance dust layer fire hazard. These findings should be taken into consideration wherever powders having melting capability are encountered in process industries or in certain public activities.

- **Keywords:** Dust layer; Fire hazard; Inclined angle; Melting fluidity; Thickness

Chenlin Wang, Yanfei Zheng, Ruikang Li, Qingrong Yin, Chunfeng Song. *Removal of cefradine by Chlorella sp. L166 and Scenedesmus quadricauda: Toxicity investigation, degradation mechanism and metabolic pathways*. Pages 632-640.

Cefradine is a broad-spectrum antibiotic employed in humans to resist bacterial infection. A large amount of cefradine was not fully utilized, which caused harm to aquatic life and aquatic environment. Herein, the toxicity, degradation and metabolic pathway of cefradine to the two microalgal species (Chlorella sp. L166 and Scenedesmus quadricauda) were investigated. The results showed that both microalgae showed excellent degradation performance for cefradine. Chlorella sp. L166 and Scenedesmus quadricauda exposed to 5 mg/L reached the highest removal rates, which were 97.27% and 98.50%, respectively. Although high concentration of cefradine inhibited the growth of both microalgal species, both microalgae showed the capacity to restore growth in high concentration of cefradine. In addition, hydrolysis and biodegradation were regarded as the main mechanisms of cefradine degradation on algae. Seven by-products of cefradine metabolism were identified by HPLC-MS and three metabolic pathways of cefradine in medium were revealed, including decarboxylation, demethylation, hydrolysis, side chain breaking and oxidation processes. These results provide a better understanding of the environmental risks of cefradine in wastewater and the efficient removal of cefradine in wastewater by microalgae.

- **Keywords:** Antibiotics; Microalgae; Biodegradation; Degradation mechanism

Jingkun Han, Dunxi Yu, Qunying Wang, Neng Yu, Jianqun Wu, Ying Liu, Lin Luo, Haoxiang Pan. *Beneficiation of coal ash from ash silos of six Chinese power plants and its risk assessment of hazardous elements for land application.* Pages 641-649.

The tremendous amount of ash produced from coal-fired power plants must be disposed and utilized in an economically and environmentally sustainable manner. This paper conducted a study on the beneficiation of silo ashes and the risk assessment for land use. Silo ash samples were collected from six Chinese power plants and segregated into five size fractions by a combination of sieving and air classification. The concentration distributions of nine hazardous elements (i.e., As, Cd, Cr, Cu, Hg, Ni, Pb, Se, and Zn) were characterized. The results show that the particle size distributions of hazardous elements in the silo ashes do not exactly agree with the generally accepted models of their release and partitioning in the boiler. Environmental risks were assessed for agricultural and development land use of coal ash, according to related Chinese standards. The results suggest that all the bulk ashes meet the requirements for development land use. Beneficially, for some coal ashes, the coarse fraction (> 10 μm) can be applied to agricultural land while the remaining fraction (< 10 μm) still complies with the standard for development land use. This work demonstrates that a simple air classification is potentially an eco-friendly and value-added approach for the full utilization of coal ash.

- **Keywords:** Coal ash; Hazardous elements; Land applications; Air classification; Risk assessment

Kaiyou Huang, Xiaoyan Wang, Wenyi Yuan, Junying Xie, Jingwei Wang, Jinhui Li. *Remediation of lead-contaminated soil by washing with choline chloride-based deep eutectic solvents*. Pages 650-660.

A promising technology has been proposed for the remediation of lead-contaminated soil by using diluted deep eutectic solvents (DESs) in this research. The DESs were synthesized by mixing choline chloride with ethylene glycol, urea, propylene glycol, glycerin and malonic acid. The experiment influences factors on the lead-contaminated soil remediation were investigated, and a response surface analysis was conducted. Scanning electron microscopy (SEM) and X-Ray diffraction (XRD) were applied to detect the mineral phase of contaminated soil before and after remediation. The changes of DESs dissolving lead nitrate (Pb(NO3)2) were analyzed by high resolution mass spectrometry (HRMS) and Fourier transform infrared spectroscopy (FT-IR). The results showed that up to 92.12% of lead could be removed from soil after washing 40 ℃ for 0.5 h. In the diluted choline chloride-malonate acid (Ch-M) solution, the carboxyl group and the hydrogen bond complex lead ions into complexes such as C3H2O3Pb, [Pb·Chcl·COOH] and [Ch·Pb]. Taking the remediation of one ton of lead-contaminated soil (14074.38 mg/Kg), it only costs $41.23 when the Pb removal rate reaches 92.12% using Ch-M as washing agent. This research provided an environmentally friendly and cost-effective remediation method for the lead-contaminated soil.

- **Keywords:** Soil washing; Deep eutectic solvents; Choline chloride; Malonic acid; Lead contaminated soil

Zheng Ting Chew, Zheng Xuan Hoy, Kok Sin Woon, Peng Yen Liew. *Integrating greenhouse gas reduction and waste policy targets to identify optimal waste treatment configurations via Carbon Emission Pinch Analysis*. Pages 661-675.

Municipal solid waste (MSW) is a persistent burden in many countries. The heterogeneous MSW characteristic requires a transition from the monotonous treatment strategy to a diversified low-carbon waste treatment configuration. Nevertheless, complex mathematical models hinder the policymakers from adopting scientific-based solutions in the decision-making process, and those models seldom link national greenhouse gas reduction targets to local waste policy targets. This study applies two approaches in constructing Carbon Emission Pinch Analysis to either optimize waste

treatment system configurations while considering greenhouse gas reduction and waste policy targets or identify the maximum possible national greenhouse gas reduction based on a waste treatment system configuration. Among the seven types of waste treatment systems studied, the carbon emission factor of material recycling is the lowest (−0.19 t CO2-e/t MSW), whereas open landfill is the highest (0.72 t CO2-e/t MSW). The proposed ten waste treatment configurations indicate a 1.0–2.2% reduction of national greenhouse gas emissions, in which the best-case configuration (i.e., carbon sink scenario) contributes to 3.64% of the national electricity consumption in 2030. This study provides a compendious comparison of waste treatment systems integrated with greenhouse gas reduction and waste policy targets for a more circular MSW management in countries facing the waste disposal dilemma.

- **Keywords:** Emission factor; Municipal solid waste; Negative emissions; Process integration; Waste management

Liang Gong, Shengnan Yang, Yifei Han, Kaiyan Jin, Lifan Lu, Yunji Gao, Yuchun Zhang. *Experimental investigation on the dispersion characteristics and concentration distribution of unignited low-temperature hydrogen release*. Pages 676-682.

The risk assessment of hydrogen-based technologies is necessary in the coming of hydrogen economic society. At present, most studies are focused on the room-temperature hydrogen (about 300 K) and cryogenic hydrogen (30–80 K), Low-temperature (200–300 K) hydrogen storage method is another storage option of hydrogen energy due to its high hydrogen storage density and less energy loss during the cooling process, however, the dispersion characteristics and concentration distribution of unignited low-temperature hydrogen during its sudden release is still unknown. In this work, a series of hydrogen release tests are performed with storage pressure at 0.5 MPa, the dispersion characteristics of unignited low-temperature hydrogen under different temperatures (200 K, 250 K and 300 K) and pinhole nozzles (1.0 mm, 1.5 mm and 2.0 mm) are analyzed. It is found that the concentration on the axis of low-temperature hydrogen jet increases with the decrease of the temperature of the hydrogen and increase of the nozzle diameter. The inverse concentration distribution with various hydrogen temperatures and different nozzle diameters by the scaled distance is obtained. The distances to some key levels of hydrogen concentration such as flammable envelope and safe distances are evaluated and the extrapolation model to other jet conditions is proposed. The results can be available for the improvement of the hydrogen safety codes and standards of low-temperature hydrogen storage.

- **Keywords:** Low-temperature hydrogen; Unignited release; Dispersion characteristics, concentration distribution; Safety distance

Rocco di Filippo, Oreste S. Bursi, Marco Ragazzi, Mariano Ciucci. *Natech risk and the impact of high-GWP content release on LCA of industrial components*. Pages 683-694.

Industrial facilities can be severely affected by natural hazards (NHs) often resulting in significant social, environmental, and economic consequences. One of the most serious consequences of Natech's events is the accidental release of hazardous chemicals. While special attention has been paid to leakage prevention of toxic, flammable, or pollutant components to date, the possible effects in terms of green house gas (GHG) emissions have not been thoroughly investigated. NH can trigger, indeed, the release of high global warming potential (GWP) compounds such as fluorinated gases, nitrous oxides and others chemicals from collapsed components and/or structures. Nonetheless, conventional approaches to integrate NHs with LCA of buildings focus mostly on the embodied carbon metric, evaluated as in the Bill of Material procedure. As demonstrated

by empirical evidence, these methods do not take into account the possible high-GWP compounds release in the case of extensive damage or collapse, which may lead to a general underestimation of the related carbon footprint. It is worth noticing that current international standards do not explicitly recommend the inclusion of these aspects in LCA procedures for structures. To cope with these issues, we introduce in this paper both the new concept of content release GHG emission potential (CGEP) and, a procedure, capable of integrating these effects with LCA. Finally, we provide some examples of industrial components characterized by a significant CGEP.

- **Keywords:** Natural hazards; LCA; Performance-based earthquake engineering (PBEE); Natech; Seismic risk

Jialong Liu, Qiangling Duan, Wen Peng, Lei Feng, Mina Ma, Shuwan Hu, Jinhua Sun, Qingsong Wang. *Slight overcharging cycling failure of commercial lithium-ion battery induced by the jelly roll destruction*. Pages 695-703.

Lithium-ion battery is the main power source of electric vehicles and hybrid electric vehicles due to its excellent properties. However, battery suffers overcharging during its use because of inconsistency among batteries, malfunction of charge control and inappropriate battery management. The failure behaviour, mechanism and diagnosis of battery under slight overcharging cycling are studied in this work. The experimental results indicate that battery capacity is approximately zero after failure. The industrial computed tomography images indicate that the jelly roll is destroyed by internal short circuit. This is the reason of battery failure. Impedances of battery increase much. The results of energy dispersive spectrometer indicate the occurrence of Al3+ ions. It means that the aluminium current collector is corroded. Finally, incremental capacity analysis and resistance estimation can be used to diagnose jelly roll destruction and detect failure battery respectively.

- **Keywords:** Lithium-ion battery safety; Overcharging failure; Failure detection; Failure diagnosis

Wei-Hsin Chen, Anh Tuan Hoang, Sandro Nižetić, Ashok Pandey, Chin Kui Cheng, Rafael Luque, Hwai Chyuan Ong, Sabu Thomas, Xuan Phuong Nguyen. *Biomass-derived biochar: From production to application in removing heavy metal-contaminated water*. Pages 704-733.

Wastewater treatment may help to reduce water shortages, whilst concurrently recover energy and nutrients, leading to some of the exploitation of important sources being offset. Compared to other approaches, wastewater purification via adsorption is highly-desirable. The reason is that with this simple and better-to-regenerate technique, heavy metals could be removed even under lower concentration of metal ions. Due to numerous advantages and tunable physicochemical properties, biochar has received most attention for the control of water contamination. This contributes to the solving ecology issues. Significantly, the link between biochar and the rehabilitation of resources should be studied, so that the role of biochar during the wastewater and environmental treatment is well-comprehended and scale-up. In this review, the biochar production from biomass through different routes and their critical properties are critically reviewed and presented. In addition, the activation methods of biochar are also presented and thoroughly compared. More importantly, the application of biochar in heavy metal removal is scrutinized. The factors that affect the heavy metal adsorption capacity and performance are critically evaluated. Finally, limitations and future perspectives for biochar production and application in the removal of heavy metal from wastewater are highlighted in this review.

- **Keywords:** Biochar; Biomass; Activation methods; Heavy metal; Adsorption behaviors; Wastewater treatment

Hang Yao, Juncheng Jiang, Bocun Li, Lei Ni, Yuqing Ni, Xinyu Yao. *Investigation of pyrolysis kinetics, mechanism and thermal stability of tert-butyl peroxy-2-ethyl hexanoate*. Pages 734-748.

Tert-butyl peroxy-2-ethyl hexanoate (TBPO), an important organic peroxide, is widely used as a polymerization initiator and curing agent in the chemical industry. Its thermal instability due to the presence of the peroxide bond may incur a decomposition reaction and cause further thermal runaway. The pyrolysis characteristics of TBPO were assessed by three advanced calorimetry techniques. The apparent activation energies under dynamic and adiabatic conditions were calculated, and critical thermal safety parameters were determined. The specific distribution of the pyrolysis products of TBPO were identified by combining thermogravimetry-Fourier transform infrared spectroscopy (TG-FTIR) and gas chromatography/mass spectrometry (GC/MS), and the most likely pyrolysis mechanism was proposed. In addition, density functional theory (DFT) was used to evaluate the activation free energy and activation free enthalpy for each step of the pyrolysis process at the B3LYP/def2-TZVP calculation level, and kinetic calculations at different temperatures were performed by using the conventional transition state theory. The theoretical simulation results were found to be in good agreement with the experimental data. The findings of this study can provide a favorable reference to forestall thermal safety accidents in the actual storage, transportation, and operation of TBPO.

- **Keywords:** Thermal runaway; Pyrolysis characteristics; Apparent activation energy; Pyrolysis mechanism; Density functional theory

Min Qin, Kexi Liao, Guoxi He, Yuanjie Huang, Minan Wang, Shijian Zhang. *Main control factors and prediction model of flow-accelerated CO2/H2S synergistic corrosion for X65 steel*. Pages 749-762.

As an important infrastructure for offshore petroleum development, submarine pipelines are the lifeline of offshore petroleum resources development. However, the medium flow containing H2S and CO2 threatens the normal production of oil fields. Based on 18 groups of orthogonal experiments, considering CO2 partial pressure, H2S partial pressure, temperature, pH, chloride concentration and liquid flow rate, the general and local corrosion rate were obtained. The corrosion products were characterized with SEM/EDS and XRD. The main controlling factors and corrosion mechanism were explored. Under the experimental conditions, CO2 and H2S were the main controlling factors of general and local corrosion. With the increase of gas partial pressure, the corrosion rate increaseed gradually. Flow accelerated the synergistic corrosion mechanism and model were established. Within the working condition range, the prediction error was less than 20%, which was better than ECE prediction model. The results can improve the integrity management of submarine pipelines.

- **Keywords:** Corrosion; H2S; CO2; Main control factors; Prediction model

Dongdong Xu, Yun Huang, Xing Jin, Tong Sun. *Synergistic treatment of heavy metals in municipal solid waste incineration fly ash with geopolymer and chemical stabilizers.* Pages 763-774.

Municipal solid waste incineration fly ash (MSWI-FA) is globally defined as hazardous waste and needs stabilization treatment. In this paper, synergistic treatment by geopolymerization and chemical stabilizers for the heavy metals in MSWI-FA was proposed, and its mechanism was further investigated. The leaching test showed that the

concentration of Cu, Cr, Cd, Ni, Zn and Pb could meet the requirement of disposal standard, with more than 99.8% been effectively stabilized while Cr and Ni were below the quantification limits. The MSWI-FA was activated in geological polymerization process and produced Al/Si-based hydration products, while the chemical stabilizers formed chelates with heavy metals, yielding double effects on the geopolymerization. Therefore, with the co-effectiveness of the two processes, most of the heavy metals were firmly stabilized in the compound structure. The developed geopolymerization procedure had potential applications for treating heavy metals in MSWI-FA.

- **Keywords:** MSWI-FA; Geopolymer; Chemical stabilizers; Heavy metals; Stabilization

P. Márquez, M.C. Gutiérrez, M. Toledo, J. Alhama, C. Michán, M.A. Martín. *Activated sludge process versus rotating biological contactors in WWTPs: Evaluating the influence of operation and sludge bacterial content on their odor impact*. Pages 775-785.

Two municipal wastewater treatment plants (WWTPs), based on activated sludge process (ASP) and rotating biological contactors (RBC) as biological treatments, were comparatively evaluated in terms of their operational conditions, bacterial content and physicochemical characteristics of their derived sludge (SL) to determine their influence on odor impact. The average values of influent wastewater flow, inlet chemical oxygen demand (COD) and COD removal efficiency were (ASP-WWTP vs. RBC-WWTP): 447 vs. 689 m3/d, 300 vs. 423 mg/L and 88.28 vs. 83.17%, respectively. Regarding the global odor emissions, ASP-WWTP and RBC-WWTP had a similar odor emission rate (11,177 ouE/s and 12,784 ouE/s, respectively), with sludge thickening and dewatering being the major sources of odor in both facilities. Proteobacteria, Bacteroidetes and Firmicutes were the three predominant phyla in both WWTPs, representing the 83% in ASP-SL and the 97% in RBC-SL. RBC-SL showed lower bacterial biodiversity than ASP-SL. The higher odor concentration from the sludge handling activities in RBC-WWTP were linked to the significative increments in the abundance of Porphyromonadaceae, Clostridiales, Lachnospiraceae (obligate anaerobe) and Moraxellaceae (aerobic) families compared to ASP-WWTP. However, when odor emissions were evaluated per equivalent inhabitant (EI), a higher value was obtained for ASP-WWTP (16.22 ouE/s·EI) compared to RBC-WWTP (6.84 ouE/s·EI).

- **Keywords:** Activated sludge process; Genomic analysis; Odor emissions; Rotating biological contactors; Sewage sludge

Haotian Ye, Wei Gao, Hong-guang Dong, Mingshu Bi. *An inherently safer development approach for thermally coupled distillation sequences: Application in hazardous chemical separation*. Pages 786-802.

Process safety is always a core issue in chemical industry, which is conventionally not taken into consideration during the conceptual design stage of a process flowsheet. Distillation handles more than ninety percent of the separation and purification tasks of hazardous chemicals and accounts for no less than forty percent of the total energy consumption. Therefore, this work presents an inherently safer synthesis framework for thermally coupled distillation sequences with structure constraints, which can efficiently quantify and optimize the inherent safety index of each column configuration in the sequence, based on State-Task Network and Dow's F&EI. To efficiently quantify the inherent safety index of each column configuration, a series of structure constraints are proposed. Within the superstructure, Hengstebeck-Underwood-Gilliland shortcut method is employed for distillation column design. Finally, two hazardous zeotropic mixture separation examples are performed to demonstrate the feasibility and validity of the proposed synthesis methodology.

- **Keywords:** Inherent safety; Thermally coupled distillation; Dow's F&EI; Optimization; Process development

Chaymae Haddaji, Karima Ennaciri, Anas Driouich, Khalid Digua, Salah Souabi. *Optimization of the coagulation-flocculation process for vegetable oil refinery wastewater using a full factorial design*. Pages 803-816.

Vegetable oil refineries wastewater poses significant challenges to treatment techniques due to its characteristic fluctuations. In this study, a full factorial design (FFD) was applied to investigate the effect of the experimental variable (pH, coagulant dose, flocculant dose, and pollutant load) for the turbidity (Y1) and COD (Y2) removal by the coagulation-flocculation process. The results showed that the linear regression models were well suited to the experimental data, with correlation coefficients R2adj of 0.96 and 0.9 for Y1 and Y2, respectively. According to the ANOVA analysis, linear effects were detected significantly for the four factors examined on turbidity and COD removal. This study has shown that coagulation-flocculation is effective for turbidity removal, regardless of the pollutant load of wastewater. Under optimal conditions using 1 g L−1 FeCl3 and 1 mL L−1 cationic polymer at a pH = 8, the turbidity removal reaches 82% and 97.5% for a low and high pollution load, respectively. In contrast, the COD removal reaches 79.5% and 58% for low and high pollution loads, respectively. These results prove that the efficiency of physicochemical treatment in organic matter removal is more effective in less polluting industrial wastewater. This strongly suggests that a physical pretreatment is a promising option for the best efficiency of coagulation-flocculation.

- **Keywords:** Coagulation-flocculation; Full factorial design; Optimization; Pretreatment; Vegetable oil refineries

Kamel Chaieb, Hisham N. Altayb, Othman A.S. Baothman, Abu-Bakr M. Gomaa, Muhammad Shahid Nadeem, Imran Kazmi, Mazin A. Zamzami. *Molecular identification of indigenous halotolerant bacteria isolated from the red sea coast applied for biodegradation of synthetic dyes and assessment of degraded metabolite toxicity*. Pages 817-838.

Three halotolerant bacteria were isolated from seawater collected along the Red sea coast, Jeddah, KSA and evaluated for their capacity to remove congo red (CR) and malachite green (MG), commonly used in paper printing and textile factories. Mixture design and response surface methodology (RSM) based on statistical design of experiments were applied to explore the region of interest and interaction between the three selected strains. Color removal were confirmed by UV–visible and Fourier transform infrared spectroscopy analysis (FTIR). Microbial enzymes related to dyes degradation were also investigated after analysis of the whole bacterial genome. Results, showed that the dye degrading strains were identified as Klebsiella pneumoniae K2, Enterobacter sp. K16b and Vibrio tritonius K20. The effect of K. pneumoniae K2, Enterobacter sp. K16b and V. tritonius K20, tested separately, induced a maximum of decolorization of 74.54%, 85.71% and 82.73% for CR and 72.67%, 74.26% and 72.73% for MG, respectively. Process optimization, showed that the higher decolorization (%) of CR and MG yields were obtained when the proportions of K. pneumoniae K2, Enterobacter sp. K16b and V. tritonius K20 were 21.34%, 56.35% and 22.30% for CR and 42.38%, 56.56% and 0.10%, for MG. Biodegradation of dyes was confirmed by UV–Vis spectrum and FTIR analysis. The phytotoxicity assay revealed that when the irrigation medium was supplemented with extract obtained from the respective microbial treated dyes solutions, seed germination, shoot and root lengths were not affected, indicating that selected strains have the ability not only to remove color but also to detoxify dyes solutions. Whole genome analysis confirms the presence of a valuable enzymes (reductase, dehydrogenase, kinase, hydrolase, transferase, catalase and, dioxygenase enzymes)

involved in chemicals degradation, suggesting that they might be useful in biological treatment of various coloured industrial effluents.

- **Keywords:** Halotolerant bacteria; Biodegradation; Mixture design; Response surface methodology; Phytotoxicity

Tianze Wang, Fuyuan Yang, Qixiang Hu, Song Hu, Yangyang Li, Minggao Ouyang. *Experimental and simulation research on hydrogen leakage of double ferrule joints*. Pages 839-846.

Owing to the scope of large-scale use of hydrogen energy in future technology, addressing safety issues like leakage and diffusion in all steps of production, storage, transportation, etc., will become inevitable. This paper focuses on the volume change of the combustible area after double ferrule joint leaks. First, a calibrated computational fluid dynamics (CFD) model was built and calibrated for accuracy through a hydrogen horizontal jet process. Second, the schlieren method was used to observe the hydrogen leakage morphology when the pipe was scratched. The CFD model was used to investigate the morphology and combustible volume changes under different wind directions and speeds. Third, critical wind speed (CWS), representing the disturbance wind speed when the combustible volume generated by the hydrogen jet was reduced to 85% of the non-disturbed environment, was proposed. Fourth, the scratch leakage behavior with the double ferrule joint placed horizontally was simulated. This research found that forced convection in the hydrogen system reduced the combustible volume produced by the hydrogen jet, and the typical value of CWS here was 1.5 m/s.

- **Keywords:** Double ferrule joint leak; Computational fluid dynamics; Critical wind speed; Schlieren method; Scratch leakage behavior

Fikret Polat. *Experimental evaluation of the impacts of diesel-nanoparticles-waste tire pyrolysis oil ternary blends on the combustion, performance, and emission characteristics of a diesel engine*. Pages 847-858.

In the present research, pyrolytic oil is obtained from the waste tire chips, and then acid washing process, clay and calcium oxide process, distillation process, and oxidative sulfur removal processes are used to improve its properties. Then it is blended into conventional diesel fuel with/without Al2O3 nanoparticles, and the performance, combustion, and emission characteristics of a single-cylinder, air cooled, and naturally aspired diesel engine are discussed in this study. Tests were performed at varying engine loads from 3 to 12 Nm with the gaps of 3 Nm under a constant engine speed of 2400 rpm. In this study, three types of fuels were tested, namely D100 (100% diesel fuel), P10 (90% diesel fuel and 10% pyrolytic oil), and P10 + 1 g Al2O3 (obtained by adding 1 g of Al2O3 nanoparticles to P10 fuel). The addition of Al2O3 nanoparticles increased the brake thermal efficiency while reducing the maximum in-cylinder pressure, heat release rate, specific fuel consumption, exhaust gas temperature, hydrocarbon emissions, NOx emissions, and CO emissions compared to other test fuels. Namely, with the addition of Al2O3 nanoparticles, BTE was improved by 4.51% and 1.59% compared to P10 and pure diesel fuel, respectively. According to this, the BSFC value increased by 4.29% for P10 test fuel and then is reduced by 2% for P10 + 1 g Al2O3 test fuel as compared with conventional diesel fuel. Compared to diesel fuel, the CO, NOx, and HC emission values deteriorated by 17.5%, 5.69%, and 18.6%, respectively, with the addition of pyrolysis oil, and these deteriorated properties were improved by 10%, 6.82%, and 13.95%, respectively, with the addition of Al2O3 nanoparticles. In the light of this study, it was observed that while waste tire pyrolysis oil worsened engine performance, emission, and combustion characteristics, these deteriorations could be improved with nano Al2O3 supplementation.

- **Keywords:** Combustion; Emission; Performance; Pyrolysis oil; Nanoparticle; Waste to energy

Yuanjun Liu, Liang Guo, Xiaomin Ren, Yangguo Zhao, Chunji Jin, Mengchun Gao, Junyuan Ji, Zonglian She. *Effect of magnetic field intensity on aerobic granulation and partial nitrification-denitrification performance*. Pages 859-867.

Magnetic field, acknowledged as a sustainable approach, is a promising method to improve the formation, stability and treatment performance of aerobic granular sludge (AGS). In this study, partial nitrification-denitrification was achieved in three AGS sequencing batch reactors (SBRs), and the effect of magnetic field intensity on AGS formation and partial nitrification-denitrification performance were investigated. 50 mT magnetic field could accelerate complete granulation time from 45 d (0 mT) to 30 d (50 mT) by promoting the settling ability of AGS and stimulating the secretion of extracellular polymeric substances (EPS). With 50 mT magnetic field, partial nitrification-denitrification in AGS was enhanced, and the removal efficiency of chemical oxygen demand (COD), NH4+-N and TN increased by 7.6%, 26.2% and 41.5% comparing with the control (0 mT). Magnetic field balanced the dominant genera Thauera, Flavobacterium, Chryseobacterium and Meganema, which further enhanced the aerobic granulation and partial nitrification-denitrification in AGS. Thus, the application of magnetic field is reliable for accelerating aerobic granulation and enhancing partial nitrification-denitrification process.

- **Keywords:** Magnetic field; Aerobic granulation; Extracellular polymeric substances; Partial nitrification-denitrification; High throughput sequencing

Thi Hai Nguyen, Seongchul Ryu, Paripurnanda Loganathan, Jaya Kandasamy, Tien Vinh Nguyen, Saravanamuthu Vigneswaran. *Arsenic adsorption by low-cost laterite column: Long-term experiments and dynamic column modeling*. Pages 868-875.

Arsenic (As) contamination of drinking water supplies is a major concern in many countries due to its large concentration in groundwater and high toxicity. In this study, batch adsorption experiments on a natural laterite adsorbent from Vietnam (NLTT) were firstly conducted, followed by four column adsorption experiments using NLTT working with synthetic water under different experimental conditions (initial arsenate As(V) concentration: 0.1 and 0.5 mg/L; bed height: 0.15 and 0.41 m). Results from the batch equilibrium adsorption study show that all three models - Sips, Langmuir, and Freundlich - fitted the experimental data very well. The Sips and Langmuir maximum adsorption capacities were 0.76 mg/g and 0.58 mg/g, respectively. At an As(V) concentration of 0.5 mg/L, adsorption breakthrough occurred at 28 h and 122 h for column heights of 0.15 m and 0.41 m, respectively. When As(V) concentration fell to 0.1 mg/L, the breakthrough times rose to 144 h and 240 h, respectively. A linear driving force approximation (LDFA) model incorporating the Sips equation was calibrated with data from the equilibrium and kinetic adsorption experiments and one column adsorption experiment (initial concentration: 0.1 mg/L; bed height: 0.15 m). The LDFA model with the calibrated model coefficients could predict the breakthrough curves and adsorption time in the three other column experiments and four household column filters used to treat As contaminated groundwater in Vietnam. The study revealed that application potential for NLTT in column adsorption studies and field trials to remove As(V) is significant despite this study having limited data. Subsequently, refining the model based on simulation of results is cost-effective, saves time and effort, and negates the need for multiple experiments to optimize filter conditions.

- **Keywords:** Arsenic removal; Adsorption column; Household filter; Laterite; Linear driving force approximation model

Ye Jiang, Da Han, Lin Yang, Zhengda Yang, Hongwei Ge, Riyi Lin, Xinwei Wang. *Improving the K resistance effectively of CeO2-TiO2 catalyst by Nb doping for NH3-SCR reaction*. Pages 876-886.

The role of Nb doping in improving anti-K poisoning ability of CeO2-TiO2 catalyst was investigated by SCR activity evaluation, BET, XRD, XPS, NH3-TPD, H2-TPR and in situ DRIFTs. The catalytic activity of the Nb-modified CeO2-TiO2 catalyst was vastly superior to that of the CeO2-TiO2 catalyst in the presence of K. The doping of Nb could enhance the BET surface area and alleviate the surface crystallinity of the CeO2-TiO2 catalyst both before and after the introduction of K. In addition, the smaller decrease in the ratio of Ce3+/Ce4+, surface chemisorbed oxygen, Brønsted acidity and redox property was observed on the Nb-modified CeO2-TiO2 catalyst in the presence of K. The results of in situ DRIFTs indicated that all of the reactions were controlled by combined E-R and L-H mechanisms on the fresh and K-poisoned catalysts. The addition of Nb could enhance the adsorption of NO and NH3, but not all NOx adsorbed species were reactive in the NH3-SCR reaction for K-poisoned CeO2-TiO2. All the above factors contributed to enhance its K-poisoning resistance of CeO2-TiO2 due to the doping of Nb.

- **Keywords:** NH3-SCR; CeO2-TiO2 catalyst; K2O; Nb doping

Mehdi Askari. *Development of a novel setup for in-situ electrochemical assessment of top of the line corrosion (TLC) and its smart inhibition under simulated conditions*. Pages 887-899.

Top of the line corrosion (TLC) is one of the main root causes for many multiphase pipeline failures in the upstream oil and gas industry. The most challenging issue for assessment of TLC in multiphase pipelines is simulating the operational conditions to find out the governing mechanisms of corrosion and its inhibition. The current work aimed to develop a novel setup for evaluating the TLC and its inhibition using the in-situ electrochemical techniques under simulated conditions. Moreover, since one of the major influencing factors in TLC is the pressure of acid gases (CO2 and H2S), an autoclave was designed to provide the feasibility of in-situ electrochemical experiments under pressurized conditions. Specialized probes were developed and placed at both the top and bottom of the autoclave to study and compare the corrosion behavior and inhibition performance at both locations. To check the function of the setup, different experiments, including electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization scanning (PDS), and linear polarization resistance (LPR) were conducted in different conditions. The performance of the system was validated by comparing the electrochemical results with weight loss coupons in autoclave and a field study in actual conditions The capability of the setup for evaluating the smart inhibition of TLC was checked with an amine-based volatile corrosion inhibitor and confirmed by EIS.

- **Keywords:** Top of the Line Corrosion (TLC); Multiphase pipelines; Autoclave; In-situ electrochemical tests; Smart inhibition

Yan Wang, Bowei Chen, Ting Xiong, Yong Zhang, Wenkun Zhu. *Immobilization of U(VI) in wastewater using coal fly ash aerogel (CFAA) as a low-cost adsorbent*. Pages 900-909.

Coal fly aerogel (CFAA), as a low-cost, recyclable and highly efficient U(VI) adsorbent, was successfully prepared. Notably, the removal rate for U(VI) of CFAA was up to 94.5% (C_0 = 10 mg L^{-1}, m/V = 1.0 g L^{-1}, T = 298 K, t = 24 h and pH = 3.0), which was much higher than previous studies. Meanwhile, the maximum removal capacity of U(VI)

on CFAA was 110.73 mg g−1 (m/V = 1.0 g L−1, T = 298 K, t = 24 h and pH = 3.0), which was nearly twice as much as untreated coal fly ash. Notable, the removal rate of U(VI) by CFAA was more than 80% after five cycles, indicating that CFAA was a recyclable adsorbent. In addition, Pseudo-second-order and Langmuir model were more suitable to describe the adsorption behavior on the surface of CFAA, meaning that the rate limiting step might be chemical sorption or chemisorption involving valency forces through sharing or exchange of electrons between sorbent and sorbate. The conclusions of SEM, FT-IR, XRD as well as XPS further illustrated that adsorption behavior for U(VI) of CFAA was mainly depended on the groups on the surface of CFAA, such as OH-, SiO- and AlO-. In conclusion, CFAA could be considered as an excellent candidate for the capture of U(VI) from wastewater.

- **Keywords:** Coal fly ash; U(VI); Immobilization; Low-cost; Complexation

Na Du, Hongting Ma, Xiaochen Yang, Kun Yang, Qingxin Zhao. *Investigation on the heat transfer and product characteristics of waste PCB recycled by a novel pilot-scale pyrolysis furnance*. Pages 910-920.

Printed circuit boards (PCBs) is a major constituent of the waste electric and electronic equipment, which represents a rapidly growing disposal problem worldwide. In order to achieve large-scale treatment of PCB, this work designed an innovative pilot-scale fixed-bed pyrolysis experiment system and proposed detailed on-site temperature measurements to quantify the impact and the delays of the temperature acceleration process. The large heat absorption of the pyrolysis reaction causes low heat transfer efficiency and significant temperature gradient along the vertical of the polit-scale furnance. Furthermore, X-ray fluorescence spectrometer, scanning electron microscope, gas chromatography–mass spectrometer and ion chromatograph were applied for the analysis of the pyrolysis product characteristics. The proportions of the phenolic compounds are 69.23%, 68.46% and 56.17% corresponding to the temperatures of 350 °C, 450 °C, and 550 °C, respectively. Moreover, the organic bromine in the pyrolysis oil was suppressed by increasing the temperature to 550 °C. The respective contents are 46.02 mg/g, 44.19 mg/g and 38.96 mg/g. The results from this study are useful to provide necessary knowledge for the design and optimisation of the industrial application of PCB pyrolysis devices.

- **Keywords:** Pilot-scale pyrolysis reactor; Printed circuit board; Temperature distribution and gradient; Heat transfer; Pyrolysis products

K.V. Yatish, H.R. Harsha Hebbar, M. Sakar, R. Geetha Balakrishna. *A comprehensive review on dairy waste-scum as a potential feedstock for biodiesel production*. Pages 921-947.

The continuous rise in crude oil prices over the last decades and crisis in feedstock availability together with food-versus-fuel debate has directed the utilization of industrial wastes for biodiesel production. Accordingly, the biodiesel or fatty acid methyl ester production has been largely explored and demonstrated with a wide variety of wastes (as feedstock materials) of which the dairy waste scum from dairy industries has been recently shown to be a viable and promising feedstock. Therefore, a critical overview on the salient features, and desirable advancements achieved with regard to dairy waste scum derived biodiesel production has become crucial. In this context, this review gives insights into the dairy scum oil methyl ester (DSOME) production, its engine feasibility and economic viability. With the scientific progress made so far by many researchers, this study compiles and analyzes numerous homogeneous, heterogeneous, nano, and bio catalysts that can be adopted for DSOME production. The feasibility of DSOME usage in engine with and without modification has also been critically discussed. An economic analysis has also been carried out to demonstrate the small-scale production of DSOME to signify its economic viability. Thus, with the possibility of demand for biodiesel, and

towards addressing the feedstock crisis, the dairy scum can be potentially developed as viable feedstock as it is abundantly and continuously available waste-material in dairy industries. This also contributes to the effective management of dairy wastes. Finally, a list of suggestions to fill the research and development gap in production, engine feasibility and economic analysis has also been proposed.

- **Keywords:** Dairy waste scum; Biodiesel; Transesterification; Engine performance; Economic feasibility

Zhesheng Hua, Qi Xin, Weijia Ren, Zhong Zheng, Feiyi Zhou, Shaojun Liu, Yang Yang, Xiang Gao. *Enhanced performance of Nb2O5 decorated RuO2/Sn0.2Ti0.8O2 for selective catalytic oxidation of ammonia*. Pages 948-957.

The ammonia slip from denitration system can result in environmental damage. Selective catalytic oxidation of ammonia (NH3-SCO) to nitrogen is one of the ideal technologies to control NH3 emission. In this work, RuO2/Sn0.2Ti0.8O2 catalysts with different Ru content and modified with Sb or Nb were evaluated for NH3-SCO. The results indicated that the RuO2&Nb2O5/Sn0.2Ti0.8O2 exhibited the similar catalytic activity and superior N2 selectivity within a wide temperature range in NH3-SCO, in comparison with RuO2/Sn0.2Ti0.8O2 and RuO2&Sb2O5/Sn0.2Ti0.8O2. Multiple techniques were used to reveal the effect of the physicochemical properties of the catalysts on the catalytic activity and N2 selectivity. For RuO2/Sn0.2Ti0.8O2, with the increasing ruthenium loading the activity enhanced together with the decline in N2 selectivity due to the high redox ability of highly dispersed ruthenium and the lack of acid sites. Particularly, in situ DRIFTS and NH3-TPD demonstrated the addition of Nb2O5 increased the quantity of acid sites, especially the Brønsted acid sites that were essential to improve N2 selectivity. During NH3 oxidation, the Brønsted acid sites promoted the activation of adsorbed ammonia to produce abundant amide intermediates (-NH2), which could directly react with the NO species to generate N2.

- **Keywords:** RuO2; Nb; Sn0.2Ti0.8O2; NH3-SCO; i-SCR

Muhammad Kashif Irshad, Muhammad Ibrahim, Ali Noman, Jianying Shang, Abid Mahmood, Muhammad Mubashir, Kuan Shiong Khoo, Hui Suan Ng, Pau Loke Show. *Elucidating the impact of goethite-modified biochar on arsenic mobility, bioaccumulation in paddy rice (Oryza sativa L.) along with soil enzyme activities*. Pages 958-967.

Contamination of paddy soils with arsenic (As) poses imminent threat to the environment and public health. This research work explored the effect of goethite-modified biochar (GMBC) on As immobilization in paddy soil and subsequent accumulation in rice grains. The results showed that the soil supplementation with GMBC significantly improved the biomass of rice plants. In addition, the GMBC application effectively decreased the As content in rice grains (0.72–0.16 mg kg−1). Compared with the control, GMBC 1.5% treatment augmented the iron plaque (Fe-plaque) buildup on rice roots and efficiently sequestered the As by 174%, and reduced its uptake in rice tissues. Soil supplementation with GMBC 1.5% greatly enhanced the activities of soil peroxidase (POD) and catalase (CAT) by 90% and 40%, respectively, compared to the control. Moreover, GMBC amendments improved the relative abundance of the soil bacterial communities and minimized the As mobility in the soil. GMBC 1.5% significantly enhanced the abundance of acidobacteria and Firmicutes by 211% and 95% while that of Chloroflexi decreased by 25%, respectively. The findings of the present investigation demonstrated that GMBC could be used as an environment-friendly approach to remediate As polluted paddy soils and minimize its accumulation in rice grains for mitigation of food security risks and protect public health.

- **Keywords:** Arsenic; Bioaccessibility; Immobilization; Paddy soil; Soil bacteria; Soil enzymes

Alibek Kopbayev, Faisal Khan, Ming Yang, Syeda Zohra Halim. *Gas leakage detection using spatial and temporal neural network model*. Pages 968-975.

Natural gas leakage can impose significant danger on a facility and its surrounding communities. Methods for early detection and diagnosis of such leakages have been developed and widely used for gas pipelines and storage tanks. Most techniques include inspection of sensor-aided mathematical models. Application of machine learning techniques to gas leakage detection has been rarely explored. In the present work, convolutional network (to model spatial likelihood of leak) is combined with bi-directional long short-term memory layer network, or BiLSTM (to model temporal dependence of leak likelihood) to perform leak detection and diagnosis. The developed model was trained and tested using sequence of concentration profiles generated using open-source simulated data. The model learned successfully to predict gas leakage and classify its size. The study also explores the flexibility of this network to perform quick detection and diagnose with the limited data. While the networks did not require parameter adjustments to achieve high prediction accuracy, further optimization is possible through data selection and pre-processing. The model needs to be further tested for wide range of leak scenarios. At its present condition, the combined application of convolutional network and BiLSTM shows promising results for early and accurate leak detection in natural gas facilities. Experimental results are needed to confirm the effectiveness of the model and data uncertainty.

- **Keywords:** Gas leak detection; Convolutional neural network; Gas leak; Safety design

Jianwei Liu, Nana Zang, Xueli Liu, Hongyu Tian, Xinyue Kang. *Bioaerosols dispersed from a typical wastewater treatment plant with a membrane bioreactor: Emission characteristics, source analysis and health risk*. Pages 976-987.

Membrane bioreactors (MBRs) have become one of the most promising technologies in wastewater treatment. This study aimed to investigate the emission characteristics, source analysis and health risk of bioaerosols generated from a wastewater treatment plant (WWTP) with an MBR throughout the entire process. The results suggested that the MBR exhibited a high concentration of bacterial bioaerosols (2921–6173 CFU/m3) and fungal bioaerosols (77–673 CFU/m3) and a high proportion of the respiratory fraction (RF) of bioaerosols. In the MBR, Halomonas, Microvirga, and Geodermatophilus and Rubellimicrobium were the dominant bacteria, and the predominant fungi were Acidea, Neophaeosphaeria, and Cryptotrichosporon. Water soluble ions (WSIs) in the bioaerosols were mainly SO42-, NO3-, Cl-, Ca2+, Na+ and NH4+, with concentrations ranging from 18.68 to 183.41 μg/m3. Temperature, relative humidity (RH) and wind speed (WS) all had different influences on bacterial bioaerosols and fungal bioaerosols. Air was the major source of bioaerosols from the MBR. Bioaerosols in the fine grid (FG) and sludge dewatering room (SDR) were from wastewater, sludge and air. Furthermore, inhalation was the greatest pathway of bioaerosol exposure. The SDR, aeration tank (AerT) and MBR showed the highest risks of bioaerosols. Thus, bioaerosols from MBRs should be sufficiently investigated, and effective controls should be set up to protect workers and residents around plants.

- **Keywords:** Wastewater treatment plant; Membrane bioreactor; Bioaerosol; Water-soluble ions; Source analysis; Health risk

Neda Ayashi, Alireza Najafi Chermahini, Mohammad Saraji. *Biomass conversion to alkyl levulinates using heteropoly acid carbon mesoporous composites*. Pages 988-1000.

With regards to the importance of biomass conversion into valuable compounds such as alkyl levulinate (AL), herein, the synthesis of butyl levulinate (BL) and ethyl levulinate (EL) from various carbohydrates (fructose, glucose, and sucrose) was studied using a series of phosphomolybdic acid (HPMo) catalysts supported on carbon mesoporous CMK-8 and CMK-3. The effect of acid loading as well as the influence of carbon mesoporous on carbohydrate conversion into ALs was investigated. Furthermore, mono lacunary phosphomolybdate catalyst supported on CMK-8 was prepared and its efficiency was compared to the optimum catalyst (CMK-HPM-50). XRD, N2 adsorption-desorption, SEM-EDX, FT-IR, TGA-DTA, and TEM analysis were performed for characterization of the synthesized catalysts. Compared to other catalysts, CMK-HPM-50 with 50% acid loading on CMK-8 showed the best results for the BL and EL production with yields of 42, 57, 66% and 53, 64, 72% from sucrose, glucose, and fructose, respectively, due to the unique 3D cubic mesostructure of CMK-8 and high Brønsted acidity of immobilized HPMo. The conversion of carbohydrates to ALs (BL and EL) was almost completed (> 98%) at all of the experiments. Various factors including, the amount of catalyst, reaction time, and reaction temperature were studied. According to the results, 50 mg of CMK-HPM-50 catalyst, 180 °C for the reaction temperature, and 3 h for the reaction time were selected as optimum conditions.

- **Keywords:** Biomass conversion; Alky levulinates; Heteropoly acid; Carbon mesoporous; Phosphomolybdic acid; Mono lacunary phosphomolybdate