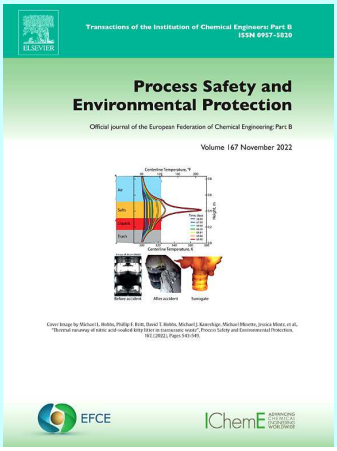
Process Safety and Environmental Protection

Rok 2022, Volume 166

October



Xinhong Li, Han Zhao, Renren Zhang. *Data-driven dynamic failure assessment of subsea gas pipeline using process monitoring data*. Pages 1-10.

Monitoring data of process variables can reflect the system condition, which can be used to perform real-time failure assessment of process operations. This paper presents a data-driven methodology for dynamic failure assessment of process operations using process monitoring data, and it is comprised of Variational Mode Decomposition (VMD) implemented with Hierarchical Bayesian Model (HBM). The monitoring data of process variables tend to be non-stationary and complex. Firstly, VMD is used to separate the noises from monitoring data to obtain the true signals. Subsequently, the failure of process operations is estimated using HBM with the true signals as the inputs. A case study of a subsea gas pipeline system is used to illustrate the methodology. It is observed that the methodology can capture the failure time of subsea gas pipeline by using raw monitoring data of process variables. It can be a useful tool to support the online failure assessment of process operations.

- **Keywords:** Condition monitoring data; VMD; HBM; Failure assessment; Subsea gas pipelines

Haojie Zhang, Chan Zhou, Hanxuan Zeng, Zhou Shi, Huiying Wu, Lin Deng. *Novel sulfur vacancies featured MIL-88A(Fe)@CuS rods activated peroxymonosulfate for coumarin degradation: Different reactive oxygen species generation routes under acidic and alkaline pH*. Pages 11-22.

A novel rod-shaped MIL-88A(Fe)@CuS featured with sulfur vacancies (SV) were constructed as heterogeneous catalysts for activating peroxymonosulfate (PMS) for coumarin (COU) degradation. A series of xMIL@CuS were obtained according to the mass content of MIL-88A(Fe) in the composites (x, wt% = 50 %, 65 %, and 80 %). Among them, 65 % MIL@CuS hold the best performance, and realized a complete COU removal (30 μM) in 7 min (0.2 g/L 65 %MIL@CuS and 0.5 mM PMS). The degradation was much more favorable in acidic initial pH than alkaline initial pH. The calculated reaction rate

constants at initial pH of 3.0, 5.0, 6.0 and 9.0 were 0.903, 0.729, 0.650 and 0.095 min−1, respectively. Electron paramagnetic resonance (EPR) analysis, radical scavenging tests and mechanism exploration indicated that the main difference in degradation under acidic and alkaline pH came from the yield of 1O2. In initial pH = 3.0 condition, SV and lattice oxygen on 65 %MIL@CuS participated in the generation of 1O2, greatly increasing the content of 1O2 (11.6 × 10−11 M) and promoting the degradation. While under initial alkaline condition (pH = 9.0), 1O2 were basically produced from the reaction between Cu(II) and PMS, resulting in a low yield (1.7 × 10−11 M) and lower degradation. Besides, 65 %MIL@CuS maintained excellent reusability with low metal ions leaching, and the degradation exceeded 98.0 % even in the fifth run. Overall, this work provided an efficient and stable activator for activating PMS to degrade refractory organics, and managed to disclose the activation mechanisms under acidic and alkaline pH.

- **Keywords:** Metal organic frameworks; CuS; Peroxymonosulfate; Sulfur vacancy; Mechanism

Shukla Neha, Neelancherry Remya, S.F. Mendes Pedro, Joris W. Thybaut, Wenes Ramos da Silva, Alberto Wisniewski. *Catalytic hydrodeoxygenation of bio-oil obtained from microwave co-pyrolysis of food waste and low-density polyethylene*. Pages 23-29.

Food waste can be a useful carbon resource when chemically recycled. While co-pyrolysis of realistic food waste (FW) has been studied, its complex upgrading is yet to be investigated. The catalytic hydrodeoxygenation (HDO) was employed for studying the pyrolysis oil generated from microwave co-pyrolysis of FW and low-density polyethylene (LDPE). More particularly, the effects of reaction temperature and time on stream were assessed in a continuous flow reactor. The combination of 48 h on stream at 200 ºC exhibited optimal performance in terms of nitro-oxygenated compounds reduction (N1–2, O1N1, O1N2 and O2N1 classes) and large oxygenated compounds classes (O7-O9) conversion into smaller ones (O1-O4). Stability analysis of pyrolysis oil showed that HDO significantly improved the properties of HDO oil (density, pH, TAN and HHV) and stabilized its properties for longer storability (60 days), i.e., after HDO at 48 h/200 ºC the oil quality had improved in terms of lower density (18 %), moisture content (88 %) and TAN (74 %) along with a higher pH and HHV (28 % and 51 %, respectively). This brings the HDO oil quality close to generic bio-oil and bio-diesel standard requirements.

- **Keywords:** Thermoconversion; Food waste; Polyethylene; Hydrodeoxygenation; Lipids

Biaojun Zhang, Yanling Wang, Hongxiang Zhu, Shaobin Huang, Jialin Zhang, Xuewei Wu, Biqing Li, Xiannian Xiao. *Evaluation of H2S gas removal by a biotrickling filter: Effect of oxygen dose on the performance and microbial communities.* Pages 30-40.

A cost-efficient and environmentally friendly biofiltration system is essential for desulfurization to recover elemental sulfur and sulfate for extensively remediating H2S. This work investigated the H2S removal capacity, accumulation of desulfurization products, sulfur balance, microbial community, and the pathway for sulfide oxidation under different O2 doses (1%, 3%, 5%, and 10%). The results showed that the removal efficiency of H2S increased from 94.1% to 100.0% with the increase of O2 dose. At 1% O2, the elimination capacity (EC) was 5.72 ± 0.33 gH2S m−3 h−1, and about 78.13% of S0-S was generated. However, with stepwise increase of O2 concentration to 10%, the EC became 6.00 ± 0.35 gH2S m−3 h−1, and SO42−-S was the dominant product at 80.39%. Furthermore, the sulfur balance was verified by calculating the proportion of sulfur compounds (S0-S, SO42−-S, and SO32−-S) and comparing the microstructure of

packing material in the biotrickling filter. Moreover, 16 S rRNA high-throughput sequencing analysis showed that the cooperation of sulfur-oxidizing bacteria in the biofiltration system was the key to the stable and efficient removal of H2S. In addition, possible reaction pathways in which H2S was transformed to S0 and SO42− were proposed.

- **Keywords:** H2S removal; Sulfur balance; Oxygen dose; Microbial community; Oxidation pathways

Shuaiyu Zhao, Jiali Huo, Rongcen Xu, Yingchun Liu, Mingju Jing, Bin Zhang. *Prevention of bund overtopping after a catastrophic tank failure accident: Effects of bund design, liquids and scale-up*. Pages 41-56.

Hazardous materials are usually stored in large tanks surrounded by bunds to prevent the disastrous consequences of catastrophic tank failure. The effectiveness of the bunds system is demonstrated by its ability to prevent liquid overtopping and withstand dynamic pressure. Therefore, this work experimentally investigates the effect of bund design parameters, including shapes, inclined angles and breakwaters, primarily on overtopping fraction, flow behavior and dynamic pressure on the bund, to provide a guideline for the effectiveness of bund parameters to reduce liquid leakage. In addition, two three-dimensional (3D) models based on the RNG k-ε and Large Eddy Simulation (LES) turbulence models were employed and systematically validated against two series of experiments to study the complex phenomenon of liquid overtopping in the bunds built according to the terrain. The overtopping fraction and dynamic pressure were studied on the petroleum products with different physical characteristics and the scale-up effect of liquid overtopping by using the RNG k-ε model. These results will contribute to the reliable design of subsequent bunds and reduce the potential risks for the safety management of tank farms.

- **Keywords:** Catastrophic tank failure; Overtopping fraction; Dynamic pressure; Bund overtopping; CFD model

Avinash Terapalli, Dinesh Kamireddi, Veluru Sridevi, M. Tukarambai, Dadi V. Suriapparao, Chinta Sankar Rao, Ribhu Gautam, Prerak R. Modi. *Microwave-assisted in-situ catalytic pyrolysis of polystyrene: Analysis of product formation and energy consumption using machine learning approach*. Pages 57-67.

Microwave-assisted catalytic pyrolysis is a prominent technology for the production of high-quality fuel intermediates and value-added chemicals from polystyrene waste. The objectives of this study were to understand the role of catalyst (KOH) on polystyrene (PS) pyrolysis. Pyrolysis experiments were conducted using a microwave oven at a power of 450 W and a temperature of 600 °C. Graphite susceptor (10 g) was used to achieve the required pyrolysis conditions. In addition, the design of experiments (DoE) with machine learning (ML) was used to understand the loading of PS (5 g, 27.5 g, and 50 g), and KOH (5 g, 7.5 g, and 10 g). The products including oil, gas, and char were collected in every experiment. The average heating rates achieved were in the range of 30–50 °C/min. The specific microwave power (microwave power per unit mass of feedstock) decreased with an increase in PS amount from 90 to 9 W/g. However, the specific microwave energy (microwave energy per unit mass of feedstock) (27–73 kJ/g) was in line with the average heating rate. The maximum yield of pyrolysis oil was found to be 95 wt%, which was obtained with a PS:KOH ratio of 27.5 g: 7.5 g. The oil yield increased from 80 to 95 wt% when the mass of the catalyst increased from 5 to 7.5 g. On the other hand, the gas yield (3–18 wt%) varied significantly and char yield (1–2 wt%) was not influenced. The yields predicted by ML matched well with the experimental yields.

This study demonstrated the potential of KOH as a catalyst for PS pyrolysis technology as the formation of aliphatic hydrocarbons in the oil fraction was significantly promoted.

- **Keywords:** Microwave; Pyrolysis; Graphite; Polystyrene; KOH; Reaction mechanism

Hui Xu, Haoran Zhang, Meng Qi, Mingqi Bai, Yunqing Xu, Lan Li, Yi Liu. *Thermal hazard evaluation of sodium dichloroisocyanurate via TG-MS, DSC, and ARC*. Pages 68-77.

Sodium dichloroisocyanurate (NaDCC) is a novel and effective material for sterilization, disinfection, and bleaching. However, the utilization of NaDCC has caused several thermal runaway incidents worldwide, raising attention to exploring its unknown thermal hazards. This paper simulated the different incident conditions to conduct a comparative study on the thermal stability and decomposition of NaDCC using thermogravimetric analysis (TGA), differential scanning calorimetry (DSC) and accelerating rate calorimeter (ARC). The gaseous products of the thermal decomposition of NaDCC were analyzed by a thermogravimetry-mass spectrometer (TG-MS). Several kinetic methods were used to calculate Ea of the pyrolysis reaction of NaDCC under different conditions. TMRad and self-accelerating decomposition temperature (SADT) were calculated based on the thermodynamic and kinetic analysis. The results of TMRad showed that the adiabatic induction period decreased significantly, and the risk of losing control enlarged with increasing temperatures. Meanwhile, by comparing the SADT of NaDCC under several common packaging materials, the chemical plastic drums should be used for packaging materials of NaDCC. The result clarifies the reason for incidents and provides the fundamentals and valuable data for safe preparation, production, transportation, and storage of NaDCC.

- **Keywords:** Sodium dichloroisocyanurate; Thermal hazard; Thermodynamic; Kinetic analysis; Thermal analysis

Fang Yang, Dandan Li, Zixian Zhang, Ling Wen, Siwan Liu, En Hu, Ming Li, Li Gao. *Characteristics and the potential impact factors of microplastics in wastewater originated from different human activity*. Pages 78-85.

To understand the characteristics and main impact factors of microplastics in wastewater at Shaanxi Province of China, the abundance, color, size and composition of microplastics in the influent and effluent of wastewater treatment plants (WWTPs) in two regions have been comprehensively studied. Three different types of wastewater have been investigated, including industrial wastewater, wastewater from urban area and wastewater from rural area. Compared with the microplastics in wastewater from industrial and urban areas, microplastics in the wastewater from rural area had a larger percentage of small particles (<0.5 mm) with bead shape. Polypropylene, polyethylene and polyethylene terephthalate were the three most abundant polymeric materials for microplastics. Furthermore, microplastics with film shape were relatively easy to be removed with the removal efficiency up to 90%. Our results have also shown that the types of wastewater, locations, population density, and treatment plant performance were all important factors influencing the potential microplastics pollution. Source control was considered as the most effective measure for preventing the microplastics pollution.

- **Keywords:** Microplastics; Physicochemical characteristics; Impact factors; Wastewater treatment plants; Removal efficiency

Qi Zhang, Lan Fan, Hetang Wang, Han Han, Zhuoqi Zhu, Xia Zhao, Yuxuan Wang. *A review of physical and chemical methods to improve the performance of water for dust reduction*. Pages 86-98.

Dust control is of great significance to industrial process safety and environmental protection. Wet dust reduction is the most commonly used dust control technology, and the physical and chemical properties of water are closely related to its dust reduction ability. In order to improve dust reduction efficiency, scholars have done much fruitful work in the physical and chemical modification of water. It is essential to summarize the progress of this research direction and shows what is lacking at present in recent years. This paper reviews the research progress on improving the performance of water for dust reduction by physical and chemical methods in the past ten years. The physical methods are mainly adopted to improve dust reduction performance in spray technologies, which include air atomization, ultrasonic atomization, magnetized water and water mist charging. And the chemical methods are mainly used to prepare dust suppression materials, which can be distinguished by single-phase dust suppressants and gas-liquid two-phase dust suppression foam. In this paper, we analyze the advantages as well as disadvantages of various methods and point out the unresolved issues. Furthermore, the development directions are proposed to provide meaningful guidance for wet dust reduction technologies.

- **Keywords:** Dust control; Water-based media; Dust reduction performance; Physical modification; Chemical modification

Xia Hu, Jiajia Wang, Tao Jin, Ziying Li, Yiu Fai Tsang, Baojun Liu. *Efficient H2O2 generation and bisphenol A degradation in electro-Fenton of O-doped porous biochar cathode derived from spirit-based Distiller's grains*. Pages 99-107.

Bisphenol A (BPA) is an endocrine disrupting chemical with high detection frequency and content, which seriously harms the ecology and human health. Spirit-based distillers' grains (DG) are solid residues produced during the brewing process, and their treatment has gotten the concern. It is an attractive effort to combine the comprehensive utilization of DG with the removal of BPA. Herein, O-doped porous biochar (OPB) was fabricated using DG as the precursor and used in an electro-Fenton (EF) system to degrade BPA. OPB exhibited a large surface area (i.e., 1432 m2/g) and doping of oxygen, which can facilitate dissolved O2 diffusion and enhance the yield of H2O2 (i.e., 3.0–15.5 mmol/L), and 20 mg/L BPA was rapidly removed by the EF system at the optimum condition (i.e., −0.5 V, pH 4, and 0.3 mM Fe2+) during 30 min with the apparent kinetic constant of 0.267/min. In addition, OPB demonstrated efficient stability in removing BPA after four cycles in the EF system. According to the results of density functional theory calculation and ultra-performance liquid chromatography–tandem mass spectrometry analysis, the three pathways were inferred to be hydroxylation, ketoneation, oxidation, and benzene ring cleavage, and then further decomposed into CO2 and H2O, and the toxicity to the environment gradually decreased with the occurrence of the reaction. This study provides a new idea for resource recovery from waste biomass to solve the problem of water pollution.

- **Keywords:** Distillers' grains; O-doped porous biochar; Electro-Fenton; BPA; Reaction mechanism

Peng-fei Zhu, Xing-fu Chen, Fu-qing Meng, Xu-bin He, Wang-hua Chen. *Thermal risk modeling and safety optimization of an arylamine diazo reaction based on PLS algorithm*. Pages 108-112.

In this study, a multi-factor reaction thermal risk model and a safety optimization method based on partial least squares (PLS) method were proposed. First, orthogonal experiments of key influencing factors were designed to obtain the correlation data between influencing factors and characteristic indicators of thermal risk. Then, the PLS method was employed to establish the reaction thermal risk model between them. Finally, this model was utilized to predict the worst-case scenario and optimize the permissible scope of influencing factors. The proposed method was applied to an arylamine diazo reaction as a representative example. The influencing factors included sulfuric acid concentration and diazonium salt concentration, while the characteristic indicator of thermal risk was the initiation temperature of adiabatic induction period of x hours (TDx). Setting TD24 > 30 °C, TD8 > 35 °C, TD4 > 40 °C, and TD1 > 45 °C as constraints, the optimal result was sulfuric acid concentration ≥ 72.8% and diazonium salt concentration ≤ 41.2%. Moreover, if 5% industrial deviation was tolerated, the optimal result was sulfuric acid concentration ≥ 76.2% and diazonium salt concentration ≤ 38.2%.

- **Keywords:** Thermal risk modeling; Initiation temperature; Multivariate analysis; Partial least squares method; Diazotization reaction

Qi Zuo, Hong Zheng, Pengyi Zhang, Yu Zhang, Baichao Zhang. *Preparation of activated carbon fibers rich in S/N/O adsorption sites for selective and efficient trace Pb(II) removal from drinking water*. Pages 113-122.

Selective and efficient removal of trace heavy metals from drinking water has been a challenging problem. Herein, we report novel activated carbon fibers rich in S/N/O multiple active sites (ACF-S/N/O) obtained by hydrogen peroxide pretreatment and 2,5-dimercapto-1,3,4-thiadiazole (DMTD) post-functionalization. The coexistence of -SH, =N-, -NH-, -NH2, -COOH and -OH functional groups in ACF-S/N/O greatly increased adsorption performance and selectivity for trace lead. The adsorbent prepared at optimum nominal mass ratio (9:11) of ACFs pretreated by hydrogen peroxide (ACF-O) to DMTD represented excellent and selective adsorption behavior for trace lead, and maximum adsorption capacity which effluent concentration met World Health Organization (WHO) standard attained 29.05 mg g−1, which was far above those of previously reported materials. Moreover, the adsorbent also exhibited rapid adsorption dynamics, superior selectivity for trace lead, and excellent adsorption performance under broad pH and concentration range, as well as in tap water. The adsorption data were well fitted to Freundlich and D-R isotherm models and pseudo-second-order kinetic model, respectively, suggesting chemical adsorption mechanism. The abundant S/N/O active sites greatly overcame mass transfer resistance of trace lead and promoted the chelation between the adsorption site and trace lead, making adsorbent exhibit excellent application prospects for drinking water purification.

- **Keywords:** Activated carbon fibers; S/N/O adsorption sites; Trace lead; Adsorption; Drinking water

Shun-xiang Shi, Si-qi Jiang, Chun-chen Nie, Biao Li, Hong-hao Chang, Xiang-nan Zhu. *Kinetic characteristics and mechanism of copper leaching from waste printed circuit boards by environmental friendly leaching system*. Pages 123-132.

Copper is one of the most important valuable elements in waste printed circuit boards (WPCBs), which can be finally recovered by hydrometallurgy. Environmentally-friendly copper leaching technology has become critical. In this study, two environmentally friendly leaching systems, namely ammonia-ammonium chloride leaching system and glycine-hydrogen peroxide leaching system, on copper leaching behavior was concerned, the influence of leaching time and leaching agent concentration on leaching rate of copper concentrate with different size was revealed. In addition, a simple but effective leaching kinetics model were proposed. The results show that with the extension of time, the leaching rate increases rapidly at first (0–10 min) and then slowly (10–25 min) until stable. The optimum leaching concentration of ammonia is 3 mol/L. For ammonia leaching system, the leaching rate increased from 76.92% to 90.05% with the decrease of particle size. Meanwhile, the leaching rate increased from 77.32% to 87.93% in the glycine leaching system. Finer particles have a larger contact area, resulting in higher leaching rates. The simple leaching kinetics model proposed in this study can accurately describe the leaching process of copper. These two environmentally friendly leaching systems can be used as substitutes for traditional inorganic acids.

- **Keywords:** Waste printed circuit boards; Metal copper; Ammonia leaching; Glycine leaching; Leaching kinetics; Leaching kinetics model

Xi Wang, Ligang Zheng, Jian Wang, Rongkun Pan, Zhanwang Shi, Jianlei Zhang, Yuxin Miao. *Experimental study on the oxygen-enriched biogas explosion characteristics by co-firing propane in a duct*. Pages 133-142.

To demonstrate the effect of propane co-firing on the explosion characteristics of the oxygen-enriched biogas, deflagration experiments were conducted in a semi-open duct. The results show that the tulip flame transforms from an existence to a disappearance with increasing oxygen fraction. The increasing brightness of the flame indicates that the increase in oxygen fraction can enhance the explosion strength and accelerate flame propagation. A clear backward motion of the burnt gas is clearly distinguished in the direct imaging of flame propagations. The propane effect is discernible when the flame evolves in a dynamic manner shortly after the flame skirt is in touch with the sidewalls. Moreover, the oxygen fraction impacts the extent of this dynamic feature and thus the magnitude of the propane effect. The laminar burning velocity SL can be singled out to forecast the flame propagation speed. The propane effect on SL and [H+OH+O]max gradually strengthens with increasing oxygen enrichment. [H+OH+O]max is well related to the fundamental properties of the mixture, such as SL, the expansion ratio, initial temperature and flame thickness, which in turn dominate flame propagations in the duct.

- **Keywords:** Biogas; Propane co-firing; Oxygen-enriched explosion; Laminar burning velocity

Yinghua Han, Qing Li, Chen Wang, Qiang Zhao. *A novel knowledge enhanced graph neural networks for fault diagnosis with application to blast furnace process safety*. Pages 143-157.

With the advent of industry 4.0, many traditional industries are moving toward automation, intelligence, and large-scale. The continuous expansion of production scale also means that the structure of industrial processes and the interactions between subsystems are becoming increas- ingly complex, which also introduced potential safety risks into the actual production. Due to the complexity and danger of the production

process, the process safety of the modern blast furnace (BF) ironmaking process is a prominent problem. In this paper, a novel fault detection and di- agnosis (FDD) framework is proposed, which can detect the abnormality and infer the root cause with no need of building an accurate mechanism model as the traditional methods. After a fault is detected, to better learn fault propagation mechanisms of the BF ironmaking process, a process knowledge model was proposed and integrated with the data-driven approaches for fault diagnosis. Then, to discover the causalities matrix of the faulty data generating procedure, a novel root cause analysis method based on Graph Neural Networks (GNN) was developed. Moreover, to accurately describe the causal interactions of faulty variables and solve the problem of the redundant edges in the causal discovery, the process knowledge constraint item was added to the GNN model to guarantee the discovered causal graph matches with the practical domain knowledge to strengthen its application in the practical industry. The experimental results on real BF data set and a bench- mark data set (The RT 580 data set) demonstrate that our algorithm not only obtains a significant improvement over other methods but also has a favorable application in the industrial process.

- **Keywords:** Fault detection; Root cause analysis; Graph neural networks; BF ironmaking process safety

Xiaopeng Li, Xiaoyan Sun, Xu Zhou, Zijie He, Kairong Lin, Xiaohong Chen, Guangming Jiang. *Fabrication of immobilized algal-bacterial beads and its application in synthetic mariculture tail water treatment*. Pages 158-165.

With the rapid expansion of the maricultural scale, the treatment of mariculture tail water (MTW) has become a focus of marine environmental protection. Meanwhile, as a cost-effective wastewater treatment technology, immobilized algal-bacterial beads (IABB) has received wide attention. The nutrients removal of wastewater by IABB is limited by the stability and strength of the beads during the treatment process. In this study, the fabrication of IABB composing Chlorella vulgaris and activated sludge with different concentration of SA (1.5%, 2.5% and 3.5% w/v) and Ca2+ (2%, 3.5% and 5% w/v) and their application in the treatment of synthetic MTW was primarily investigated. The SA concentration has significant impact on the characteristics of IABB. Specifically, 2.5% of SA resulted in the formation of IABB with the best homogeneity, chemical and mechanical stability. Ca2+ concentration affect the nutrient removal efficiency during MTW treatment. The IABB fabricated under the conditions of 2.5% SA and 2% Ca2+ showed the highest removal efficiency of NH3-N, TP and COD within the 48 h of experiment, i.e. 66.7 ± 3.2, 81.0 ± 2.8 and 90.7 ± 1.9%, respectively. Therefore, the application of IABB offers promising prospects for MTW treatment and marine environmental safety.

- **Keywords:** Immobilized algal-bacterial beads; Mariculture tail water; Algal-bacterial symbiosis system; Chlorella vulgaris; Activated sludge

Jing Dang, Ni Zhang, Meng Qi, Mingqi Bai, Hui Xu, Zhongxu He, Lan Li, Chi-Min Shu, Yi Liu. *Study on thermal stability and thermal decomposition mechanism of 1,1-di-tert-butyl peroxy-3,3,5-trimethyl cyclohexane through adiabatic calorimeter and theoretical approach*. Pages 166-176.

Organic peroxides (OPs) readily demonstrate oxidising and self-reactive characteristics that can easily cause fire and explosion. Information regarding the thermal stability and other properties of OPs should be provided to industries that use these materials to avoid unexpected thermal decomposition in the workplace. The target substance in this study, 1,1-di-tert-butyl peroxy-3,3,5-trimethyl cyclohexane (TMCH), is commonly used in the

chemical industry, and scholars have considered its applications in the aerospace sector in the last two decades. Because of different conditions in the chemical and aerospace industry, parameters measured under the previous conditions leave unforeseen thermal risks. The thermal behaviour and runaway pathway of TMCH, especially under adiabatic conditions, were investigated using experimental and theoretical computation methodologies. Differential scanning calorimetry, thermogravimetric analyser, and adiabatic accelerating calorimeter were applied for the thermokinetic constants of TMCH. Experimental results indicated that TMCH could release heat and gas when decomposed, with a high potential explosion hazard. Molecular simulation calculations can compensate for the measurement restrictions of instruments. The peroxy bond dissociation energy of TMCH was amended by basis set superposition error correction calculations. The analysis determined the thermal runaway reaction pathway of TMCH and evaluated the formation mechanism of the transition state defined by the intrinsic reaction coordinate. The main reason for TMCH mass loss caused by heating was the release of CO2 and ethane gas. This paper confirmed experimental results by molecular simulation with thermodynamic constants. The study results can be used as a reference for the loss prevention and control of TMCH in more potential engineering applications.

- **Keywords:** Organic peroxides; Adiabatic accelerating calorimeter; Molecular simulation; Runaway reaction; Intrinsic reaction coordinate

Van Cam Thi Le, Mahshab Sheraz, Eunsil Kang, Huyen Ngoc Ly, Hien Duy Mai, Woo Ram Lee, Choong-Gon Kim, Seungdo Kim. *Four-in-one multifunctional air filter using copper coordination polymer particle decorated fibre for efficient pathogen removal and indoor air treatment*. Pages 177-188.

This paper introduces a multifunctional air filter with a strong ability to trap and disinfect pathogens and absorb particulate matter (PM), the volatile organic compound (VOC), and CO2. This study demonstrates a facile and eco-friendly synthesis of copper coordination polymer particle (Cu-CPP)-decorated non-woven fibre filters (Cu-CPP/NWF) via an in situ growth dip-coating method. Their multifunction potentials in air pollution treatment are also assessed. The Cu-CPP/NWF filter media showed a remarkable performance for air treatment, with 100% disinfection efficiency against airborne E. coli bacteria (2 × 106 CFU mL−1) in 45 min, superior PM removal efficiency (quality factor 0.299 Pa−1), excellent p-xylene adsorption capacities (1.19 mmol/g) and high potential CO2 uptake capacities (19.81 cm3/g). A Cu-CPP can work as an antibacterial agent and an adsorbent component, thus offering many applications. The rational integration of Cu-CPP can substantially enhance the filtration efficiency via electrostatic interaction, while most commercial air purifiers rely on dense fibrous filters. This study provides valuable insight into developing a multifunctional and reusable air filter proven to be a life-saving product for public health protection.

- **Keywords:** Multifunctional air filter; CO2 capture; P-Xylene adsorption; PM2.5 collector; Antimicrobial; Copper coordination polymer particle

Kulbir Singh, Manvi Kaushik, Mohit Kumar. *Integrating α-cut interval based fuzzy fault tree analysis with Bayesian network for criticality analysis of submarine pipeline leakage: A novel approach*. Pages 189-201.

Submarine pipelines are the major transportation mode of marine oil and gas resources. Because of submarine pipeline damage, the leakage of oil and gas will result the serious consequences such as environmental disasters, fires and explosions, and huge economic losses. There are variously internal and external factors that initiate spill accidents of oil and gas. To prevent and mitigate such accidents, risk analysis is an efficient way. Fault

tree analysis is an effective tool to identify failure causes and perform the risk assessment. In fault tree analysis, it is presumed that all basic events are statistically independent and have precise occurrence probabilities. In the case, when probability data of basic events of system fault tree are unavailable or imprecise, the concept of fuzzy set theory and expert elicitation is used to obtain qualitative data. In the quantification of qualitative data, experts' knowledge is used which may raise issues such as incompleteness, imprecision, and lack of consensus. In the process to minimize the uncertainty, expert's opinions are aggregated and updated to the posterior possibilities using the prior observations. Bayesian networks have the advantages of representing the dependencies of events, updating probabilities, and dealing with uncertainties. In this research paper, a novel methodology is proposed by combining fuzzy fault tree analysis and Bayesian network to obtain updated prior possibilities of basic events and top event of system fault tree when new information are available. The main contributions of this research are: weakest t-norm based arithmetic operations on fuzzy numbers are employed for less uncertainty accumulation during the process; weakest t-norm and α-cut based similarity aggregation method is developed to evaluate the possibilities of basic events and top event in system fuzzy fault tree analysis; the obtained prior possibilities are then updated using fuzzy Bayesian network; criticality analysis is executed using the posterior possibilities of basic events and top event. Further, a case study of leakage in submarine pipeline is discussed to demonstrate the applicability and effectiveness of the proposed methodology. The obtained results are then compared with the pre-existing results which shows the validity and applicability of the proposed method.

- **Keywords:** α-cut interval; Bayesian networks; Fault tree analysis; Weakest t-norm; Submarine pipeline leakage

Shennan Zhou, Zhongqi Wang, Qizhong Li. *A conceptual framework integrating numerical simulation with system theory based method for quantitative explosion process hazard analysis*. Pages 202-211.

Explosion is a significant threat to chemical process safety, which often occurs suddenly with a wide range of impact, resulting in catastrophic disasters. Predictions of explosion hazards are required for regional safety assessment and disaster resilience enhancement of chemical industrial parks (CIPs). This paper, therefore, aims to develop a conceptual framework for systematically analyzing explosion evolutions and quantifying the potential hazards by combining system-theoretic process analysis (STPA) method with numerical simulation. The proposed framework consists of 5 steps: (i) establishment of hierarchical safe control structures (SCSs) of important chemical processing zones in the CIP, (ii) computational fluid dynamics (CFD) modeling for potential explosion evolutions in each zone by changing the examined parameters randomly, (iii) development of a convolutional neural network (CNN) prediction model through constant self-learning of CFD pressure field data, (iv) comprehensive assessment of blast damage by incorporating the outputs of the above numerical models into existing evaluation methods, (v) identification of unsafety control actions and causes, and safety constraints for the improvement of SCSs. Provided with monitoring data, the developed analysis architecture can predict explosion process hazards and recommend appropriate safety strategies in real time. This would service the multi-level requirements for explosion prevention and protection, supporting better-informed decision-making. The paper describes the concepts and implementation process of the method as a first step.

- **Keywords:** Explosion hazard analysis; Explosion flow field prediction; STPA; CFD simulation; Convolutional neural network

Mingxiang Liu, Wei Chen, Jiawei Fu, Anqi Wang, Mingmei Ding, Lei Zhang, Le Han, Li Gao. *Hyaluronic acid-modified nanofiltration membrane for ultrahigh water permeance and efficient rejection of PFASs*. Pages 214-221.

Emerging contaminants (ECs) in water, such as per- and polyfluoroalkyl substances (PFASs), require more efficient separation technology for water treatment. Although nanofiltration (NF) has exhibited the potential to remove small organic molecules, enhancing water permeance without sacrificing the rejection of the membrane is still a big challenge. Herein, we fabricate a novel thin-film composite (TFC) membrane by introducing a hyaluronic acid (HA) interlayer. The hydrogen bonds between HA and amine monomers depress the mass transfer of piperazine, which is beneficial for constructing a thinner and denser polyamide (PA) layer. As a result, we finally obtained a novel TFC membrane with a PA layer with a more negative surface, reduced thickness, crumpled structure and higher degree of cross-linking. Moreover, the obtained TFC membrane exhibits an excellent water permeance of 29.53 L m−2 h−1 bar−1 and high rejection for Na2SO4 (94.90 %) and perfluorohexane sulfonic acid (PFHxS) (93.4 %). In light of the low cost and ease of performance, our study proposes a new, green strategy for fabricating TFC NF membranes for environmental water treatment that could feasibly be extended to industrial applications.

- **Keywords:** Thin-film composite; Per- and polyfluoroalkyl substances; Hyaluronic acid; Polyamide membrane

Tengfei Chen, Jo Van Caneghem, Jan Degrève, Jan Berghmans, Filip Verplaetsen, Maarten Vanierschot. *Comparison between a numerical model and the classic thermal explosion theories for the calculation of the minimum ignition temperature of dust clouds*. Pages 222-231.

A numerical model for the calculation of the minimum ignition temperature (MIT) of dust clouds is compared with the classic Semenov and Frank-Kamenetskii thermal explosion theories. The numerical model is developed based on the MIT testing equipment: Godbert-Greenwald furnace. The Semenov theory for uniform temperature system is exploited for the MIT calculation of a single dust particle (MITP). The Frank-Kamenetskii theory for a uniform system with temperature gradient is modified for the MIT calculation of a dust cloud (MITC). At stoichiometric dust concentration with infinite dust cloud residence time, two horizontal asymptotes are discovered along with the variation trend of the numerical ignition temperature against ignition delay time. The higher asymptotic temperature is only discovered for metal dusts. This temperature is almost identical to the MITP value with the Semenov theory. On the other hand, the lower asymptotic temperature for both metal and organic dusts almost equals the calculated MITC value with the Frank-Kamenetskii theory. Thus, there is good agreement between the numerical model and the classic thermal explosion theories. This study can provide reference for the theoretical prediction of the MIT of dust clouds.

- **Keywords:** Minimum ignition temperature; Dust clouds; Numerical model

Masih Soleymani, Farzaneh Sadri, Susanna Zhang, Ahmad Ghahreman. *The role of thiosulfate and sulfite in gold thiosulfate electrowinning process: An electrochemical view*. Pages 232-240.

In this study, electrochemical and analytical techniques are employed to explore the effect of thiosulfate, sulfite, and a mixture of thiosulfate-sulfite in the electrolyte on the gold electrowinning process. The open circuit potential (OCP) analysis showed negative potential shifts from − 0.02 V (in the electrolyte containing Au-TS (E1)) to − 0.21 V, − 0.33 V, and − 0.42 V in the presence of thiosulfate oversupply (electrolyte E2), sulfite

(electrolyte E3), and thiosulfate-sulfite mixture (electrolyte E4). The linear sweep voltammetry (LSV) results exhibited − 0.4 V potential shift by the addition of sulfite to the gold-thiosulfate electrolyte, attributing to the formation of Au(S2O3)(SO3)25- as the most stable gold complex. Based on chronoamperometry (CA) and atomic absorption spectrometer (AAS) results, sulfite could control the kinetics and thermodynamics of gold reduction reactions by minimizing undesired cathodic side reactions such as thiosulfate decomposition or water reduction, resulting in purer gold deposition, elimination of colloidal sulfur, and a more efficient EW process. The presence of thiosulfate accelerated the kinetics of the gold reduction reaction. However, adding sulfite to the electrolyte stabilized the kinetic about 10 times faster. SEM and EDS analysis depicted the morphological changes in the deposited gold layer from different electrolytes during CA, showing that thiosulfate oversupply results in the formation of a greater number of smaller grains by accelerating the nucleation process, while sulfite addition led to the formation of a smoother and more uniform gold layer on the cathode surface.

- **Keywords:** Gold deposition; Electrochemical reduction; Electrowinning; Sulfite; Thiosulfate

Yongyong Jia, Yulong Wang, Risheng Zhuo, Fang Lou, Shikui Jin, Pengxiang Zhao. *Research on the safety control technology of gob-side entry in inclined thick coal seam*. Pages 241-248.

To study the safety control technology of the gob-side entry in an inclined thick coal seam, the asymmetric deformation characteristics and control mechanism of the gob-side entry in an inclined thick coal seam were analysed by combining theoretical analyses, numerical simulations and field monitoring with the prototype of a gob-side entry in a deep inclined thick coal seam in a high gas mine in Xinjiang. The research results showed that the deformation of the solid coal gang and top plate is more intense than that of the narrow coal pillar gang and bottom plate. Combined with the asymmetry of deformation surrounding rock, the gob-side entry safety control technology based on a high prestressing high-strength anchor support and a reinforced support by inclined anchor cables in key areas (a zero-displacement area within the narrow coal pillar and an intense deformation area of the solid coal gang angle) is proposed. Reasonable the gob-side entry support parameters were further determined via numerical simulation experiments, and a reasonable anchor length, row spacing and spacing to maintain the stability of the gob-side entry were obtained as 2200 mm, 800 mm and 800 mm, respectively. Engineering practice showed that the adoption of the new support technology can effectively control the asymmetric large deformation of the solid coal gang and top plate, which can maintain the stability of the gob-side entry for a long period of time and ensure the safe and efficient production of coal resources in the mine.

- **Keywords:** Inclined thick coal seam; Gob-side entry; Flac3D; Asymmetric deformation; Surrounding rock control

Maria Cristina Collivignarelli, Marco Carnevale Miino, Giacomo Cillari, Stefano Bellazzi, Francesca Maria Caccamo, Alessandro Abbà, Giorgio Bertanza. *Estimation of thermal energy released by thermophilic biota during sludge minimization in a fluidized bed reactor: Influence of anoxic conditions*. Pages 249-256.

Thermophilic biological fluidized bed reactors operating in aerobic/anoxic alternate conditions proved to be a feasible solution for sewage sludge minimization. However, to date, no data about energy released by thermophilic biota (ThBio) are available in literature. This work aims to estimate specific thermal energy released by ThBio highlighting the influence of daily anoxic conditions. A pilot-scale reactor (1 m3) was fed continuously with mesophilic sewage sludge and monitored for more than four months

and a thermophysical model was applied to estimate thermal energy released by ThBio (kT,biota and kT,COD). Results suggested that the increase of daily anoxic time stimulated COD removal (92.7 ± 1.3 % vs. 81.3 ± 4.9 %, with 6 h and 0 h of daily anoxic time, respectively). The thermal energy released by ThBio was strictly dependent on anoxic conditions. In fact, increasing anoxic conditions from 0 h d−1 to 6 h d−1, kT,biota and kT,COD reduced from 1.8 ± 1.3 Mcal kg−1VS kg−1COD and 26.6 ± 13.7 Mcal kg−1COD to 0.5 ± 0.1 Mcal kg−1VS kg−1COD and 15.6 ± 4.2 Mcal kg−1COD, respectively. Although, biological mechanism responsible of this behaviour is not completely clear, this work can serve as reference for future studies about the optimization of conditions to maximize thermal energy release from ThBio during organic substance degradation alternate aerobic/anoxic, in view of subsequent energy recovery.

- **Keywords:** Thermophilic biota; Sewage sludge minimization; Biota metabolism; Energy balance; Organic substance degradation; Advanced biological process

Andong Yu, Xinyi Zhao, Min Hua, Xuhai Pan, Melis Duyar, Xinmiao Liang, Yiming Jiang, Juncheng Jiang, Chi-Min Shu. *Process hazard evaluation and thermal runaway prediction for styrene polymerization initiated by peroxide-azo composites*. Pages 257-268.

Styrene is an important monomer for synthetic resins, ion exchange resins and synthetic rubber. Styrene polymerization requires the use of initiators to increase the reaction rate, with composite initiators showing promise for increased reaction rates. However, increased reaction rates in polymerization, if uncontrolled, can lead to thermal runaway with disastrous consequences. Numerous runaway incidents have been documented, indicating inadequate awareness of the thermal hazards of polymerization reactions. This study focuses on determining via calorimetric techniques the thermal hazards of styrene polymerization using azodiisobutyronitrile (AIBN) and tert-Butyl peroxybenzoate (TBPB) composite initiators. Differential scanning calorimetry (DSC) is employed to investigate the thermal decomposition properties of composite initiators with varying composition. Non-isothermal experiments and adiabatic experiments are used to determine the thermal hazard parameters including initial exothermic temperature and heat release of styrene polymerization. The risk of secondary reactions is evaluated by reaction calorimetry (RC1e) and product thermogravimetric analysis (TGA). Key safety parameters of the exothermic reaction, such as the onset temperature, heat release, time to maximum rate under adiabatic condition as well as activation energy, are presented. The results show that the thermal hazard of the polymerization reaction is lowest when the ratio of AIBN to TPPB in the composite initiator is 1:1. In this scenario, the temperature reached by the uncontrolled reaction does not provoke the decomposition of the products, yet the runaway consequences are still unacceptable. This work provides extensive data as a reference for the process optimization of styrene polymerization from the perspective of safety.

- **Keywords:** Styrene polymerization; Thermal runaway; Composite initiators; Calorimetric techniques; Thermal hazard

Fenghui Wu, Ye Liu, Guangfei Qu, Ruosong Xie. *High value-added resource treatment of antimony tailings: preparation of high-strength lightweight foam concrete materials*. Pages 269-278.

The continuous exploitation of global mineral resources leaves ever increasing tailings, which leads to the accumulation of antimony tailings and causes antimony pollution accidents. The complex chemical composition and associated harmful elements of antimony tailings limit their large-scale consumption and high-value comprehensive utilization. To realize the solidification/stabilization of antimony tailings with heavy metals and achieve large-scale high-value utilization, in this paper, high-strength and

lightweight concrete materials based on antimony tailing powder were prepared by using antimony tailing powder as the main raw material, and cement clinker, activator, coagulant and foaming agent as the supplements. In this manner, the performance of high-strength and lightweight concrete materials were investigated and optimized in terms of mechanical properties, waterproofing properties, micromorphology, etc. The experiment results show that the decrease of the compressive strength and apparent density of the specimen slurry is due to the increased amount of antimony tailing micronized powder. Additionally, the influence of different foaming agents on the material is significant. With the addition of antimony tailing of 50% and H2O2 of 0.6% into the cementitious material of PC42.5, the material presents optimal high-strength and lightweight performance. Moreover, the compressive strength at 28 d reaches up to 36.2 MPa, and the dry apparent density is as high as 1449.2188 kg/m3. In addition, the optimal system has been optimized in terms of waterproof performance. Softening coefficient of the composite with optimized composition was increased by 55.1%, reaching 0.86, which is sufficiently high for waterproof application.

- **Keywords:** Antimony tailings; Solidification/Stabilization; Leaching toxicity; Lightweight concrete

Jinlong Zhao, Qingyuan Zhang, Xiang Zhang, Jianping Zhang, Rui Yang, Yu Lu. *Experimental study and thermal hazard analysis of large-scale n-heptane pool fires under sub-atmospheric pressure*. Pages 279-289.

Tank farms are commonly used for storing large quantities of liquid fuels. The design, construction, operation, and maintenance of a tank farm must be in accordance with standards/codes applicable to specific countries. Existing codes on the design of storage tank farms are largely based on tests performed at standard atmospheric pressure and associated thermal hazard analysis. Studies based on small-scale experiments, however, have shown that the burning behavior and associated radiation impact of liquid fuels could be substantially affected by the reduced pressure at high altitude. In this study, large-scale n-heptane pool fire experiments with different pool diameters were carried out at sub-atmospheric pressure to firstly investigate their burning characteristics. Subsequently, specific fire scenarios for the cases under both standard and sub-atmospheric conditions were selected for assessing and comparing their thermal hazards. The experimental results showed that the burning rate at sub-atmospheric pressure is reduced, whereas the flame height is increased. Correlations for both the burning rate and flame height including the pressure effect were proposed and validated against the experiment data in this and existing studies obtained at different pressure conditions. The flame radiative fraction was found to decrease exponentially with the pool diameter. The thermal hazard analysis showed that whilst the thermal hazard at sub-atmospheric pressure is lower than that at standard atmospheric pressure, this difference gradually reduces with increasing tank diameter. The present results not only are important in understanding the effects of pressure on the burning characteristics of large-scale pool fires but provide guidance on the applicability and limitations in the use of design codes developed for standard atmospheric pressure for plateau regions.

- **Keywords:** Pool fire; Sub-atmospheric pressure; Burning characteristics; Thermal hazard; Tank farm codes

Locksley F. Castañeda, Oscar Coreño, José L. Nava. *Simultaneous removal of arsenic, fluoride, and hydrated silica from deep well water by electrocoagulation using hybrid Al-Fe electrodes*. Pages 290-298.

This paper deals with the simultaneous removal of arsenic, fluoride, and hydrated silica (HSi) from natural deep well water (26 μg L−1 As, 1.65 mg L−1 F−, 160 mg L−1 HSi, 0.3 mg L−1 PO43−, pH 7.5, and conductivity 450 μS cm−1) by electrocoagulation (EC). An up-flow EC reactor made up of an eight-cell stack using aluminum and iron plates as

sacrificial electrodes in horizontal mode was used. The influence of the mean linear flow velocity ($1.2 < u < 4.8\,cm\,s{-}1$) and current density ($3 < j < 5\,mA\,cm{-}2$) applied to the EC reactor on the removal efficiency of As, F−and HSi was systematically examined. The best electrocoagulation trial was obtained at $j = 5\,mA\,cm{-}2$ and $u = 1.2\,cm\,s{-}1$, producing an aluminum and iron coagulant dose of 33.73 and 68.4 mg L−1, respectively, attaining residual concentrations of arsenic ($CAs = 0.02\,\mu g\,L{-}1$) and fluoride ($CF{-} = 0.88\,mg\,L{-}1$) below the World Health Organization (WHO) guideline ($As < 10\,\mu g\,L{-}1$ and $F{-} < 1.5\,mg\,L{-}1$). The residual HSi concentration was $CHSi = 33\,mg\,L{-}1$, with electrolytic energy consumption and total operating cost of EC of 2.07 KWh m−3 and 0.29 USD m−3, respectively. The SEM-EDS, FXRD, XRD, FTIR, and Raman analyses of the Al-Fe flocs evidence the formation of iron silicates and aluminosilicates formed by the reaction between iron and aluminum with silica, respectively, and the existence of iron oxides and iron oxyhydroxides. The arsenic was removed by adsorption on aluminum and iron aggregates, while fluoride substitutes a hydroxyl from aluminum flocs.

- **Keywords:** Electrocoagulation; Arsenic; Fluoride; Groundwater; Aluminum-iron electrodes

Saeed Balafkandeh, Seyed Mohammad Seyed Mahmoudi, Ehsan Gholamian. *Design and tri-criteria optimization of an MCFC based energy system with hydrogen production and injection: An effort to minimize the carbon emission*. Pages 299-309.

The threat of rapid depletion of fossil fuel reserves and the discharge of pollutants due to the depletion of these resources has had catastrophic consequences for the ecosystem. Using efficient energy systems, waste heat recovery from these systems, and decreased carbon dioxide emission cycles is one approach to averting this looming threat in this context. It is proposed in this paper to utilize the electricity generated by the bottoming absorption power cycle to create hydrogen for use in a molten carbonate fuel cell-based energy system. The system is called near-zero carbon since the efficient waste heat utilization allows maximum hydrogen and minimum hydrocarbon fuel use. The concept of the near-zero carbon cycle is being explored from the viewpoints of technology, economics, and the environment. It is necessary to do multi-criteria optimization to establish the optimum operating point of the system under consideration to reduce costs and CO2 emissions while simultaneously increasing efficiency. A parametric analysis is performed to discover the important design parameters that impact the system's performance under consideration. Included among the factors under investigation are the fuel utilization factor (Uf), current density (J), stack temperature (Tstack), and the steam to carbon ratio (rsc). Upon investigation, it was discovered that the suggested system had an energy and exergy efficiency of around 66.21% and 59.5%, respectively. According to the findings of the exergy analysis, the MCFC and afterburner ranked highest in terms of exergy destruction (93.12 MW and 22.4 MW, respectively). The tri-objective optimization findings also reveal that the most optimal solution point has an exergy efficiency of 59.5%, a total cost rate of 11.7 ($/GJ), and CO2 emission of 0.58 ton/MWh.

- **Keywords:** Carbon neutral system; Sustainability; Fuel cell; Multi-criteria optimization; Hydrogen production; And injection

Christian Schweizer, Chad V. Mashuga, Waruna D. Kulatilaka. *Investigation of aluminum dust cloud dispersion characteristics in an explosion hazard testing device using laser-based particle and flow diagnostics*. Pages 310-319.

Monitoring the dust cloud dispersion process inside testing equipment like the MIKE3 minimum ignition energy device is useful for assessing the ignitability characteristics of

different dust materials. However, it is difficult to comprehensively capture the relevant micro-scale particle properties and macro-scale flow behavior of a dust cloud dispersion using a single measurement method. Thus, the objective of this work is to combine two complementary laser diagnostic techniques to obtain quantitative particle and flow properties from dust clouds in the MIKE3 glass tube. For this experiment, thirty repeated runs for each method were conducted using small (15-mg) aluminum powder samples. No ignition electrodes are included in the test geometry to establish a baseline flow configuration for the glass tube, although measurements are still made at the characteristic time delay and location of ignition tests. The first technique, digital in-line holography (DIH) is used for three-dimensional micro-scale particle diagnostics, yielding particle number ($n = 78 \pm 20$), size ($\overline{D} = 18.9 \pm 0.6\,\mu m$), and three-component velocity ($\overline{v}x = 0.05 \pm 0.05\,m/s$, $\overline{v}y = 0.60 \pm 0.09\,m/s$, $\overline{v}z = -0.07 \pm 0.16\,m/s$) measurements. The second laser diagnostic technique, particle image velocimetry (PIV), is used for macro-scale flow diagnostics, yielding two-dimensional flow velocity and vorticity vector field measurements. Particle sizes are observed to follow a lognormal distribution ($\mu = 2.89$, $\sigma = 0.31$), and a discrepancy between in-situ and ex-situ sizing results is identified for particle sizes larger than ~55 µm. Two-dimensional particle velocities follow a Weibull distribution ($\theta = 0.86$, $\beta = 2.12$), and reasonable agreement is found between the DIH and PIV velocity measurements.

- **Keywords:** Particle size; Particle velocity; Flow velocity; Dust cloud characterization; Dust explosion; Laser diagnostics

Christian Schweizer, Chad V. Mashuga, Waruna D. Kulatilaka. *Investigation of niacin and aluminum dust cloud ignition characteristics in an explosion hazard testing device using high-speed imaging*. Pages 320-327.

Experimental investigations of dust explosions in standard industrial testing equipment such as the MIKE3 minimum ignition energy (MIE) testing device are promising ways of producing fundamental insights into dust cloud ignitability. However, advanced experimental methods must be developed to characterize the dust cloud ignition and combustion behavior of various types of dust. In this work, high-speed broadband and species-specific chemiluminescence imaging diagnostics are implemented to explore similarities and differences between organic and metal powder ignition kernel development. A selected set of 600-mg niacin ($\varphi = 2.9$) and aluminum ($\varphi = 1.6$) powder samples were dispersed in the air and ignited using a high-voltage spark inside a standard MIKE3 device. The resulting broadband flame emission was recorded at 4 kHz using a high-speed camera for the first 10 ms after the spark. For the niacin sample, species-specific chemiluminescence emissions from excited-state hydroxyl (OH*) and methylidyne (CH*) radicals were also recorded at 4 kHz and 1 kHz, respectively. The flame kernel in each image frame was detected using an intensity thresholding algorithm and tracked throughout the video sequence, yielding quantitative size, position, and velocity measurements of the evolving flame kernel during the first 10 ms after the ignition spark. For the niacin sample, a continuous and non-uniform reaction zone composed of burning particle clusters and excited-state radicals was observed. The niacin flame kernels grew from 5 mm to 17 mm with an initial velocity of 5 m/s. Conversely, an intensely bright reaction zone and discrete burning particles near the flame kernel boundary were observed in the aluminum sample. The aluminum flame kernels grew from 7 mm to 10 mm with an initial velocity of 3 m/s. The niacin and aluminum flame kernels traveled 7–11 mm away from the central spark gap and slowed down to 1 m/s by the end of the 10-ms period. This time-resolved imaging study, when coupled with previously reported three-dimensional particle and flow field data prior to the arrival of the ignition spark, sets the foundation for an improved multi-physics understanding of the initiation of dust cloud ignition and explosion processes.

- **Keywords:** Spark ignition; Flame kernel development; High-speed imaging; Dust cloud combustion; Dust explosion

Shuo Chen, Yiyuan Rong, Lingli Tu, Zebin Yu, Hongxiang Zhu, Shuangfei Wang, Yanping Hou. *Coupling the bioanode and S-scheme CuO/CdS quantum dots photocathode for chlortetracycline degradation: Performance, mechanism and microbial community*. Pages 328-340.

The quantum dots (QDs) modified S-scheme CuO/CdS photocathode was fabricated and integrated with a bioanode in the bio-photoelectrochemical system (BPES) for chlortetracycline (CTC) degradation under simulated solar irradiation using NaHCO3 as buffer. The S-scheme CuO/CdS QDs heterojunction was demonstrated by work function calculation and electron spin-resonance spectroscopy (ESR) test. The optimized CuO/CdS QDs photocathode exhibited great photocatalytic activity toward CTC degradation, due to its unique small-size effect, efficient light absorption, and efficient carriers separation and transfer. Results of ESR test demonstrated that hydroxyl (·OH), superoxide (·O2-) and carbonate radicals (·CO3-) could be produced by the photocathode, and they all contributed to CTC degradation. The degradation rate of CTC by BPES was 1.29 times that of the unilluminated system (86.8% vs 67.1%), and the maximum current density was 2.3 times (3.42 vs 1.48 A/m2). The dominant bacterial species in the CTC degradation of BPES were Pseudomonas and Acinetobacter. Possible mechanism and pathways of CTC degradation were proposed. This study advances the development of BPESs for antibiotics degradation.

- **Keywords:** Bio-photoelectrochemical system; S-scheme CuO/CdS quantum dots photocathode; Chlortetracycline degradation; Carbonate radicals; Microbial community

Boqiang Lin, Chongchong Zhang. *Forecasting carbon price in the European carbon market: The role of structural changes*. Pages 341-354.

Examining and analyzing the role of breakpoints in carbon price prediction can help people better understand the carbon market's structural changes to carry out technological predictions. However, the current carbon price prediction models lack comprehensive utilization of structural breakpoints. Then, a hybrid forecasting model is proposed by combining the Bai&Perron test, Iterated Cumulative Sums of Squares algorithm (ICSS), wavelet transform, and long short-term memory neural network (LSTM). According to the results, there are fifteen breakpoints in the EU allowance (EUA) carbon price. And the breakpoints can improve the prediction accuracy of the proposed model by 10–20 %. The ICSS algorithm is superior to the Bai&Perron test in detecting the breakpoints and improving the prediction accuracy. Compared with other benchmark models, the proposed hybrid model has the best prediction accuracy. We suggest that two types of breakpoints information could be accounted for in future prediction models.

- **Keywords:** Carbon price prediction; Bai&Perron test; Iterated Cumulative Sums of Squares algorithm (ICSS); Wavelet transform; Long short-term memory neural network

Peng Wu, Yaqin Hu, Yaping Zhang, Kai Shen, Yiliang Liu, Goubo Li, Hongqiang Yang, Sheng Wang. *Enhanced activity and N2 selectivity for manganese oxides catalysts modified with transition metals: Mechanism and N2O formation pathways*. Pages 355-367.

Various transition metals were employed to enhance the catalytic performance and N2 selectivity of Mn-based catalysts. The modification of Fe and Cu promoted the low-temperature activity, while the Al-modified catalyst displayed the highest N2 selectivity

close to 100 %. The characterization results proved that the content of Oβ and Mn4+ were increased after adding transition metals. N2 selectivity experiments revealed that the reduction of NO to N2O and the oxidation of NH3 to N2O did not occur. The product of NH3 oxidation was only N2. Combined with the results of the in-situ DRIFTS experiments, it was proposed that N2O was generated from the decomposition of NHNO and NH4NO3 in the SCR reaction. The poor N2 selectivity of the unmodified catalyst was related to the existence of inactive N2O22- species on the surface, while the high content of active NH2- species on the Mn0.1Ho0.005Ce0.015Al0.01/TiO2 catalyst enhanced its catalytic activity and N2 selectivity. In addition, the results also revealed that only the E-R mechanism existed on the unmodified catalyst, while both the E-R and L-H mechanism were activated after the transition metal modification.

- **Keywords:** SCR catalyst; Transition metal; N2 selectivity; N2O formation; In-situ DRIFTS study

Maria A. Zoran, Roxana S. Savastru, Dan M. Savastru, Marina N. Tautan. *Cumulative effects of air pollution and climate drivers on COVID-19 multiwaves in Bucharest, Romania*. Pages 368-383.

Over more than two years of global health crisis due to ongoing COVID-19 pandemic, Romania experienced a five-wave pattern. This study aims to assess the potential impact of environmental drivers on COVID-19 transmission in Bucharest, capital of Romania during the analyzed epidemic period. Through descriptive statistics and cross-correlation tests applied to time series of daily observational and geospatial data of major outdoor inhalable particulate matter with aerodynamic diameter ≤ 2.5 μm (PM2.5) or ≤ 10 μm (PM10), nitrogen dioxide (NO2), ozone (O3), sulfur dioxide (SO2), carbon monoxide (CO), Aerosol Optical Depth at 550 nm (AOD) and radon (222Rn), we investigated the COVID-19 waves patterns under different meteorological conditions. This study examined the contribution of individual climate variables on the ground level air pollutants concentrations and COVID-19 disease severity. As compared to the long-term average AOD over Bucharest from 2015 to 2019, for the same year periods, this study revealed major AOD level reduction by ~28 % during the spring lockdown of the first COVID-19 wave (15 March 2020–15 May 2020), and ~16 % during the third COVID-19 wave (1 February 2021–1 June 2021). This study found positive correlations between exposure to air pollutants PM2.5, PM10, NO2, SO2, CO and 222Rn, and significant negative correlations, especially for spring-summer periods between ground O3 levels, air temperature, Planetary Boundary Layer height, and surface solar irradiance with COVID-19 incidence and deaths. For the analyzed time period 1 January 2020–1 April before and during each COVID-19 wave were recorded stagnant synoptic anticyclonic conditions favorable for SARS-CoV-2 virus spreading, with positive Omega surface charts composite average (Pa/s) at 850 mb during fall- winter seasons, clearly evidenced for the second, the fourth and the fifth waves. These findings are relevant for viral infections controls and health safety strategies design in highly polluted urban environments.

- **Keywords:** COVID-19 disease; Outdoor air pollutants; 222Rn; Aerosol Optical Depth (AOD); Climate variables; Synoptic meteorological circulation

Song Jiang, JinYuan Li, Sai Zhang, QingHua Gu, CaiWu Lu, HongSheng Liu. *Landslide risk prediction by using GBRT algorithm: Application of artificial intelligence in disaster prevention of energy mining*. Pages 384-392.

Geological disasters on the slopes of open-pit mine dumps in energy extraction fall into the category of mine production process safety. For the mine safety, it is crucial to accurately predict the landslide risk of open-pit mine dumps. In order to prevent landslide geological disasters in open-pit mine dumps under the effect of heavy rainfall,

this study establishes a fast and accurate landslide risk prediction model for open-pit mine dumps based on machine learning (ML). Given the actual geological conditions and rainfall of the slope of an open-pit mine dump in Shaanxi Province, Geo-Studio software is used to calculate the factor of slope safetyunder different states, and the gradient boosting regression tree (GBRT) algorithm model is used to predict the factor of slope safety. The comparison with the prediction results of different algorithms shows that the GBRT model has the highest prediction accuracy; meanwhile, the GBRT model predicts the factor of safety (FOS=1.283) for the bench slope of the dumps under the rainfall intensity (q=87 mm/d) of the "20-year rainstorm recurrence period", and its error is smaller than that calculated by the numerical simulation analysis (FOS=1.289). Therefore, the GBRT model has better applicability in predicting the safety factors of open-pit mine dumps slope under the effect of heavy rainfall, which is of great significance to realize the early warning of landslide risk in open-pit mine dumps.

- **Keywords:** Open-pit mine dump; GBRT; Slope stability; Factor of slope safety; Landslide risk prediction

Zhikang Deng, Yongtao Cheng, Jinyao Zhu, Lie Yang, Zulin Zhang, Li Wu. *Electricity generation and enhanced thiacloprid biodegradation in microbial fuel cells using microalgae biocathode*. Pages 393-401.

Thiacloprid (THI), as a commonly used neonicotinoid, is frequently detected in environmental media, posing a potential threat to the environment and organisms. In this study, microalgae fuel cells (MFCs) with Chlorella sp. as cathode and wastewater (with sludge) as anode were constructed to remove THI (10, 20 and 50 mg/L) while generating bioelectricity. The results showed that, comparing with the open-circuit condition, the generation of bioelectricity (closed-circuit) significant enhanced the removal of THI by 13.14–32.47%. The presence of low concentration of THI (10–20 mg/L) did not significantly affect the accumulation of Chlorella sp. biomass, while high concentration THI (50 mg/L) strongly depressed its biomass. It was also found that high concentration THI caused obvious oxidative damages (MDA) to Chlorella sp., although SOD activity was upregulated. Both the highest THI removal efficiency (%) and stable bioelectricity voltage (202 mV) occurred at the low THI concentration (10 mg/L). Seven degradation products of THI were identified and the oxidation of the thiazole ring was the main detoxification way of THI. Additionally, toxicity evaluation also showed that the toxicity of degradation products were lower than THI. This study implies that MFCs could be a promising application, coupling pollutants removal, bioenergy generation and biomass production.

- **Keywords:** Microalgae; Neonicotinoid; Toxicity; Transformation pathway

Akintomiwa O. Esan, Siwaporn M. Smith, Shangeetha Ganesan. *A non-conventional sustainable process route via methyl acetate esterification for glycerol-free biodiesel production from palm oil industry wastes*. Pages 402-413.

In the present study, a sustainable and environmentally safe process was utilized for production of biodiesel free of glycerol via methyl acetate esterification by employing the beneficial usage of palm oil industrial waste products. A non-conventional novel approach was then investigated for the esterification process using methyl acetate as the esterifying agent in the presence of solid acid catalyst prepared via impregnation on spent bleaching earth as catalyst support. The new solid acid catalyst was synthesized by calcination and sulfonation of the spent bleaching earth. The catalyst was characterized via Hammett Indicator, X-ray Fluorescence, Thermogravimetric Analysis, X-ray Diffraction, Nitrogen adsorption-desorption analysis, and Ammonia-temperature programmed desorption techniques. Optimization study was carried out for reaction

parameters such as reaction temperature (60–110 °C), catalyst amount (2–14 %), PFAD/MA molar ratio (1:3–1:18) and reaction time (1–6 h). The maximum free fatty acid conversion of 89.89 % was obtained at optimized reaction conditions: catalyst amount 12 w/w%, reaction time 3 h, reaction temperature 100 °C and PFAD/MA molar ratio 1:12. A plausible mechanism for the esterification of palm fatty acid distillate using methyl acetate in the presence of the synthesized acid catalyst has also been proposed. This study also ascertained the effectiveness of methyl acetate as a suitable alternative esterifying agent for esterification of palm fatty acid distillate.

- **Keywords:** Glycerol-free biodiesel; Free fatty acids; Bleaching earth; Methyl acetate; Optimisation

Yuxuan Xing, Jiansong Wu, Yiping Bai, Jitao Cai, Xiaoping Zhu. *All-process risk modelling of typical accidents in urban hydrogen refueling stations*. Pages 414-429.

With the rapid development of the hydrogen industry, an increasing number of hydrogen refueling stations (HRSs) are being built in urban areas with a high density of buildings and population. As a kind of emerging clean fuel, hydrogen is also highly flammable and explosive. So, the risk of multiple accidents in urban HRSs has attracted more and more concern. In this paper, an all-Process Hydrogen Accident Risk Assessment (PHARA) model that combines event tree analysis, fuzzy Bayesian network (FBN), HyRAM, and Probit model is proposed. Based on sensitivity analysis and influence strength analysis of FBN, the critical hazards of hydrogen refueling stations are identified. The risk management priority is determined by comparing the comprehensive risk value of each functional unit of HRSs. Then, the HyRAM-based quantitative consequence analysis is carried out for the high-risk unit, and the flammable zone, fatality zone, and relative safe distances of jet fire and explosion are given in a standardized urban hydrogen refueling station. The proposed PHRAR model can provide technical support for decision-makers to prevent accidents, control risk, and optimize the layout of HRSs.

- **Keywords:** Hydrogen refueling station; Risk assessment; All-process of accidents; Fuzzy Bayesian network; Probit model

Nadir Yilmaz, Stephen M. Davis. *Diesel blends with high concentrations of biodiesel and n-butanol: Effects on regulated pollutants and polycyclic aromatic hydrocarbons*. Pages 430-439.

Despite advances in alternative energy production (including electric vehicles and hydrogen fuel cells), fossil fuels remain ubiquitous and an ongoing threat to the environment. Alternative biofuels such as biodiesel and n-butanol have garnered substantial attention in recent years as additives to fossil diesel as a means to control emissions such as nitrous oxides (NOx) and carbon monoxide (CO). In addition, as biodiesel and alcohols do not contain aromatic hydrocarbons in their chemical structures, they provide potential additional advantages for reducing toxic emissions, including polycyclic aromatic hydrocarbons (PAHs); however, this is often only demonstrated for relatively low blend ratios (<20 %). In this study, the effects of neat diesel, waste oil biodiesel, and n-butanol blends on engine function, regulated, and unregulated emissions were investigated for blends containing 50/50 vol% diesel/biodiesel (D50B50), 50/25/25 vol% diesel/biodiesel/n-butanol (D50B25Bu25), and 50/50 vol% diesel/n-butanol (D50Bu50), in addition to neat standard road diesel (D100) and waste oil derived biodiesel (B100). In these blends NOx was reduced by up to 28.1 % relative to D100 for loads above idle, while increasing exhaust gas temperatures up to 33.5 % and increasing unburned hydrocarbons (HC) and CO by up to 84.2 % and 93.8 %, respectively. Measured against neat diesel, biodiesel and the diesel-biodiesel-butanol blend reduced PAH toxicity by up to 46.4 %, while diesel-biodiesel and diesel-butanol blends showed an increase up to 14.3% and 504%, respectively, due to higher concentrations of 5-ring

PAHs. It has been concluded that in addition to fuel aromaticity, other factors such as fuel properties affecting the diesel combustion process (i.e. cetane number), can cause PAH formation.

- **Keywords:** Diesel; Biodiesel; N-butanol; Diesel engine; Regulated emissions; PAHs

Enara Fernandez, Maria Cortazar, Laura Santamaria, Maite Artetxe, Maider Amutio, Gartzen Lopez, Javier Bilbao, Martin Olazar. *Tuning pyrolysis temperature to improve the in-line steam reforming catalyst activity and stability*. Pages 440-450.

This study analyzes the two-step process of biomass pyrolysis and in-line steam reforming for the production of H2. In order to evaluate the effect of the volatile composition on the commercial Ni/Al2O3 catalyst performance and stability, biomass pyrolysis step was conducted at different temperatures (500–800 °C). The analysis of the deactivated catalysts has also allowed identifying the main bio-oil compounds responsible for catalyst decay (coke precursors). Pyrolysis temperature allows modifying the composition of the volatile stream that is subsequently reformed at 600 °C. An increase in pyrolysis temperature to 800 °C improves considerably the production of both H2 and gaseous stream at the initial reaction stages, reaching values of 12.95 wt% and 2.23 Nm3 kg−1, respectively. Catalyst stability is also considerably improved when pyrolysis temperature is increased due to the lower bio-oil yield and its different composition at high temperatures. Coke was the main cause of catalyst deactivation. Besides, the nature of the coke deposited is influenced by the composition of the pyrolysis volatiles, with encapsulating coke being formed by the adsorption and subsequent condensation of all hydrocarbons (oxygenated and non-oxygenated ones) preferably at low temperatures, whereas filamentous coke is formed when the concentrations of CO and light hydrocarbons in the volatile stream are increased at 800 °C.

- **Keywords:** Pyrolysis temperature; Biomass; Conical spouted bed reactor; Hydrogen production; Steam reforming

Anfu Guo, Dekun Kong, Xiaoyan Zhou, Peng Qu, Shaoqing Wang, Jianfeng Li, Fangyi Li, Liming Wang, Yingbin Hu. *Evaluation of material reuse degree in additive manufacturing by the improved resolution coefficient grey correlation method*. Pages 451-460.

With the rapid development of additive manufacturing (AM), materials used in AM increase year by year, generating a large amount of discarded waste materials. Some of these waste materials are hazardous to the environment and the human body. Facing this problem, it is crucial to reduce material usage in AM technologies by recycling. Up until now, extensive attentions have been attracted on material reuse/recycling in AM technologies, however, comparisons of material reuse degree (MRD) are still lacking. Aiming at addressing MRD issues, we developed an improved resolution coefficient grey correlation (IRCGC) method to evaluate MRD in four representative AM technologies, including fused deposition modeling (FDM), stereolithography (SLA), selective laser sintering (SLS), and laminated object manufacturing (LOM). In such an IRCGC method, a grey correlation optimization model was established and a combined analytic hierarchy process and entropy weight method was employed to obtain weights. Afterwards, MRD in 4 AM technologies were assessed by an evaluation system and then were clustered using data analysis software. Experimental results show that among the 4 AM technologies, the FDM technology demonstrated the highest MRD, whereas, the SLA technology exhibited the lowest MRD. The SLS and the LOM AM technologies are classified into the good level.

- **Keywords:** Additive manufacturing; Material reuse degree; Combined analytic hierarchy process and entropy weight method; Improved resolution coefficient grey correlation method

Ding Zhang, Liang Ma, Linjing Zhang, Yichen Zhang, Yingfa Song, Shenwen Fang. *Process optimization and mechanism of oil-based drilling cuttings treatment based on hydrophilic deep eutectic solvent*. Pages 461-468.

Oil-based drilling cuttings (OBDC) are hazardous waste, oil removal treatment must be done before they are re-utilized. Winsor I microemulsion (composed by microemulsion phase and remaining phase) cleaning is one of oil removal methods. However, there are many surfactants in the Winsor I microemulsion, which result in high cleaning cost and high possibility of surfactant contamination. In this paper, hydrophilic deep eutectic solvent (DES) and mineral oil were used to replace the microemulsion phase and remaining phase in Winsor I microemulsion, respectively, and a low-cost and surfactant-free cleaning agent was formed. The recommended DES was the mixture of choline chloride, methanol, and water with a molar ratio of 1:2.5:3, and the best cleaning agent was the mixture of DES and mineral oil with a mass ratio of 3:1. The recommended cleaning process was that added the OBDC into cleaning agent with a mass ratio of solid to liquid of 1:3, and stirred at room temperature for 100 min. At this condition, the oil content of OBDC reduced from 14.57 wt% to 1.34 wt%. In addition, the cleaning mechanism was discussed. The DES has low surface tension and good wetting property, which is similar with the microemulsion.

- **Keywords:** Chemical cleaning; Deoiling; Microemulsion

Feng Ma, Tong Zhu, Sai Yao, Haoyu Quan, Kuo Zhang, Baorui Liang, Youzhao Wang, Yaonan Zhu, Chaoyue Zhao, Zhenning Lyu. *Coupling effect of high temperature and thermophilic bacteria indirectly accelerates the humification process of municipal sludge in hyperthermophilic composting*. Pages 469-477.

Due to its high treatment efficiency and environmental friendliness when used to treat organic waste, hyperthermophilic composting (HC) has attracted extensive attention in recent years. However, it is still unclear how HC accelerates the degradation and humification process of organic matter. This study investigated the effects of high temperature and thermophilic bacteria on the degradation and humification of organic matter during HC. In the process of HC and conventional composting (CC), total organic carbon content decreased by 30.76 mg/g and 18.50 mg/g, while humic acid carbon content increased by 2.26 mg/g and 1.41 mg/g, respectively. These results showed that HC accelerated the humification process by enhancing the degradation of organic matter and the production of humic acid compared to CC. Redundancy analysis revealed that the rapid humification process of HC was related to high temperature and thermophilic bacteria. Thermophilic bacteria accelerated the degradation of organic matter in the high temperature stage, and the degradation products provided sufficient substances for the humification reaction in the low temperature stage, thereby accelerating the humification reaction. In conclusion, the coupling effect of high temperature and thermophilic bacteria indirectly accelerated the humification process. This work contributes to understanding the humification mechanism of HC.

- **Keywords:** Hyperthermophilic composting; High temperature; Humification Process; Organic matter degradation; Thermophilic bacteria

Larissa Pinheiro de Souza, Flávio Olimpio Sanches-Neto, Giberto Mitsuyoshi Yuki Junior, Bruno Ramos, Arlen Mabel Lastre-Acosta, Valter

Henrique Carvalho-Silva, Antonio Carlos Silva Costa Teixeira. *Photochemical environmental persistence of venlafaxine in an urban water reservoir: A combined experimental and computational investigation*. Pages 478-490.

The photochemical behavior of venlafaxine (VNX) in surface water was investigated using a hybrid theoretical-experimental-kinetic modeling approach. In addition to the direct photolysis quantum yield, the rate constants of the reactions between VNX and reactive photo-induced species (hydroxyl radicals, HO·; singlet oxygen, 1O2; and triplet excited states of chromophoric dissolved organic matter, 3CDOM*) in sunlit water were measured under simulated solar radiation using competition kinetics. To elucidate possible degradation products, first-principles calculations were applied, followed by toxicity estimation by quantitative structure-activity relationship (QSAR) calculations. Furthermore, kinetic simulations of VNX persistence in an urban water reservoir of the São Paulo Metropolitan Region, Brazil, were performed. The results indicate low direct photolysis of VNX, with ΦVNX = (1.06 ± 0.18) × 10−2 mol Einstein−1. The measured values of the second-order reaction rate constants are kVNX, 3CDOM* = (3.98 ± 0.28) × 109 L mol−1 s−1 and kVNX,1O2 = (2.09 ± 0.17) × 107 L mol−1 s−1, which are lower than kVNX, HO·obs = (6.92 ± 0.37) × 109 L mol−1 s−1 and kVNX, HO·theo = 4.98 × 109 L mol−1 s−1. O-desmethylvenlafaxine, the most thermodynamically stable metabolite predicted by theoretical calculations, revealed potentially greater toxicity and, therefore, higher environmental risk to aquatic ecosystems. The estimated half-lives for VNX range from 9 to 62 days, depending on the season, local weather conditions and water quality parameters, the effects of which can be satisfactorily simulated with the aid of the modified photochemical fate model proposed in this work.

- **Keywords:** Antidepressant drugs; Competition kinetics; Computational chemistry; Photochemical fate; Toxicity; Kinetic simulations

Chaoya Zheng, Jianchao Liu, Yuanfei Cai, Chenyang Jing, Runren Jiang, Xiqiang Zheng, Guanghua Lu. *Pharmaceutically active compounds in biotic and abiotic media of rivers receiving urban sewage: Concentrations, bioaccumulation and ecological risk*. Pages 491-499.

Pharmaceutically active compounds (PhACs) are recognized as posing health risks to aquatic ecosystems. The occurrence characteristics and ecological effects of 15 PhACs were investigated in the multiphase media of Yangtze River (Nanjing area, China) during wet and dry seasons. All 15 PhACs were detected in the traditionally dissolved phase, suspended particulate matter, sediment and fish, with total concentrations of PhACs (ΣPhACs) of 64.75–366.20 ng/L, 18.50–69.40 ng/g, 3.29–23.30 ng/g and 0.00–176.44 ng/g, respectively. Ibuprofen (IPF), roxithromycin (ROX) and caffeine (CFI) were the dominant PhACs in all of the environmental media. As the main carrier for PhACs, the colloids contributed 8.60%– 77.04% of PhACs in the traditionally dissolved phase, and distribution coefficients (log Kcol=6.38–7.95) of PhACs in colloidal phase were significantly higher than those in SPM and sediment. The bioaccumulation potential of ΣPhACs in the wild fish tissues was generally in order as follows: brain > liver > kidney > gill > blood > intestines > muscle > bile, which was positively correlated with their log Kow. The concentrations of CFI, ROX and IPF in the muscle, gill and liver can be predicted by their log Kow and pollution levels in the blood, and the concentrations of PhACs in the muscle of benthic fish were much higher than those in pelagic fish. The bioaccumulation factors of ROX, fluoxetine and bezafibrate in intestines, brain and blood showed strong enrichment capacity (>5000). In the risk assessment, the acute risk level of PhACs to aquatic organisms decreases gradually with the trophic level, while the trend of chronic risk was the opposite. The chronic mixture risk of PhACs to fish was > 1 at all sampling sites, 59.79% of mixed risk quotient were provided by clofibric acid, diclofenac,

erythromycin and ketoconazole. These results indicated that PhAC can cause harmful health effects to sensitive organisms both individually and mixedly.

- **Keywords:** Pharmaceutically active compounds; Urban rivers; Environmental media; Bioaccumulation; Ecological risk

Hongyan Sun, Ruyuan Jiao, Qinxue Yang, Junjie Yu, Dongsheng Wang. *Aggregation and settling characteristics of particulate matter and DOM in a southern China reservoir: Influence of hydraulic conditions and dosing methods*. Pages 500-511.

For the in-situ treatment process of landscape waters, ponds, reservoirs and other water bodies, there is a significant deviation between the experiment results and the actual treatment effect due to volume amplification effect. Therefore, this study systematically explored the influence of hydraulic conditions, dosing frequency, dosing intervals of coagulant, and coagulant dilution multiples on the removal efficiency of particulate and organic matter on a large scale to precisely simulate the practical treatment situation. Results showed that dosing intervals and dosing frequency played an important role in the aggregation and settling process of particulate matter by influencing the energy barrier between particles, while hydraulic conditions affected the structure and settling characteristics of flocs. The overall trend of the total organic matter was consistent with that of particulate matter. However, only the freshly formed aluminum hydroxide precipitates had adsorption activity to humic substances. The adsorption could be completed rapidly so that hydraulic conditions had no influence on the aggregation process of humic substances. While during stirring and aging process, humic substances was found to be released due to the polymerization and crystallization of aluminum precipitates. From the results of pilot tests, a treatment strategy was implemented for a reservoir in southern China and the ideal treatment effect was achieved. This study provided theoretical foundation and design guidance for the in-situ coagulation treatment of landscape waters, ponds and reservoirs.

- **Keywords:** In-situ coagulation; Particulate matter; Organic matter; Hydraulic conditions; Particle sedimentation

Komal Desai, Swapnil Dharaskar, Jalaja Pandya, Satyam Shinde, Vinay Vakharia. *Experimental investigation and validation of ultrasound-assisted extractive/oxidative desulfurization of oil using environmentally benign ionic liquid*. Pages 512-523.

Owing to the increasing use of oil and global air production, a comprehensive development toward producing ultra-clean fuels is increasing daily. One can use some of the most integrated techniques to make ultra-pure oils. The ultrasound-assisted extractive/oxidative desulfurization process possesses appropriate characteristics concerning the oxidant-ionic liquid (IL) system. 1,3-dimethylimidazolium dimethyl phosphate was synthesized, characterized, and used in the UEODS process as a catalyst/extractant. The desulfurization efficiency of 97% and 68% is obtained in the cases of model oil and base oil, respectively. Furthermore, two machine learning models are compared and found to be in good concordance with the experimental observations to validate the experimental findings. Density functional theory proved that the IL has more affinity towards dibenzothiophene sulfone than dibenzothiophene. It also demonstrated that the aromatic rings of IL and S-compounds have CH- π, π-π, and hydrogen bonding interactions. The IL was recycled and reused for ten cycles.

- **Keywords:** Ionic liquid; Ultrasound-assisted extractive/oxidative desulfurization; Density functional theory; Machine learning; Dimethylimidazolium dimethyl phosphate

Yan Cui, Jianghong Liu, Beihua Cong, Xin Han, Sumiao Yin. *Characterization and assessment of fire evolution process of electric vehicles placed in parallel*. Pages 524-534.

Electric vehicle (EV) fire accidents induced by the thermal runaway of li-ion batteries are increasingly frequent, and the fire dynamics of EVs parked in rows are still unclear. Hence the fire evolution process and characteristics of two parallel placed EVs were studied by analyzing the burning behaviors and thermal fields. The fire source was the battery pack of a battery electric vehicle (BEV). Results showed that the precursor to the BEV fire was the emission of white smoke from the chassis. Flames did not appear until the accumulated smoke exploded, and they engulfed both the EVs. The flame switched between momentum and buoyancy control on the vehicle scale. The maximums of the length and duration of the jet fires were determined. The maximum temperature of the EV fire was consistent with that of internal combustion engine vehicle (ICEV) fires, but the flame spread faster between the EVs compared to ICEVs. Pragmatic methods were proposed to quantify the fire evolution rate. The heat effect of the EV fire on humans was also quantitatively evaluated. These results provide a fundamental understanding of fire rules in a high EV concentration scenario.

- **Keywords:** Full-scale fire experiment; Electric vehicle; Lithium-ion battery; Thermal runaway; Fire characteristic

Syed Saif Ali, Sharif Zamir, AR Shakeelur Raheman, Khursheed B. Ansari, Muhammad Abdul Qyyum, Mohammed K. Al Mesfer, Mohd. Danish, Mohd Shariq Khan, Ala'a H. Al-Muhtaseb. *Current progress in thermochemical conversion of plastics into jet-fuel hydrocarbons and recommendations for COVID-19 waste management*. Pages 535-557.

A vast amount of plastics are produced globally to comply with human needs. Additionally, the COVID-19 pandemic enabled an extreme rise in single-use plastic, creating an extra burden on plastic waste handling and promoting environmental pollution. Thermochemical conversion of plastic wastes into liquid hydrocarbons would be promising in this context. Numerous literature showed plastic-to-liquid hydrocarbon fuel formation; however, jet-fuel grade hydrocarbons generation from plastics is rarely assembled and hence become the focus of the current review. Reportedly, 200 – 600 °C reaction temperature, 10 bar hydrogen pressure, 12 hrs retention time, and 0.13 catalyst-to-feed ratio produced jet fuel from plastics; albeit, it remained system-specific, including batch and continuous processes. Critical evaluation of several plastics to jet-fuel techniques suggested research attention in (i) complete plastic conversion into the plastic-derived oil, (ii) catalyst selection and new design enabling aliphatic/aromatics selectivity within the product mixture, (iii) mechanistic understanding of plastic to jet-fuel processes (with and without catalyst), and (iv) catalyst recyclability studies. Thermal degradation under microwave, hydrothermal liquefaction, pyrolysis, methanolysis/hydrogenation, thermal cracking/co-hydrogenation, and aqueous phase hydrodeoxygenation are possible routes for plastic to jet-fuel conversion. Catalytic pyrolysis could be a promising for plastic/COVID-19 thermochemical conversion into jet fuel, and biomass-derived catalysts may replace the expensive metal-based catalysts.

- **Keywords:** Environmental protection; Plastics waste minimization; Thermochemical conversions; Catalyst; Batch and Continuous Operation; Aliphatic hydrocarbons

Alaa K. Ibrahim, Gaber Abuzaid Ismail, M. Abdewahab Badr, Mai M. Badr. *Incorporating of landfill leachate in fired-clay bricks manufacturing: An experimental study*. Pages 558-564.

Fired clay- brick industry consumes around 386 liters of water per 1000 bricks. Landfill leachate is considered an environmental burden. Therefore, this study aimed to use untreated landfill leachate instead of water in fired clay-brick to save water consumption and eradicate landfill leachate problems. Two types of landfill leachate were used instead of water, old and fresh leachate. They were characterized before use. Their water content was 90.9 and 95.8, respectively. Green brick was successfully manufactured without any deformation, cracking, or failure during brick molding, drying or burning. The produced fired clay- brick met the Egyptian standard requirements in terms of compression strength, water absorption, and efflorescence. It also met the environmental protection and consequently public health concerns in terms of heavy metal leaching. Recourses conservation, environmental pollution control, cost-saving, and production of standard products are the main benefits of this research work.

- **Keywords:** Landfill leachate; Old leachate; Fresh leachate; Green brick; Fired-clay brick

Xing Xin, Faisal Javid, William A. Anderson, José G.B. Derraik, Trudy Sullivan, Yvonne C. Anderson, Saeid Baroutian. *Hydrothermal deconstruction of single-use personal protective equipment: process design and economic performance*. Pages 565-573.

Increased demand for single-use personal protective equipment (PPE) during the COVID-19 pandemic has resulted in a marked increase in the amount of PPE waste and associated environmental pollution. Developing efficient and environmentally safe technologies to manage and dispose of this PPE waste stream is imperative. We designed and evaluated a hydrothermal deconstruction technology to reduce PPE waste by up to 99% in weight. Hydrothermal deconstruction of single-use PPE waste was modelled using experimental data in Aspen Plus. Techno-economic and sensitivity analyses were conducted, and the results showed that plant scale, plant lifetime, discount rate, and labour costs were the key factors affecting overall processing costs. For a 200 kg/batch plant under optimal conditions, the cost of processing PPE waste was found to be 10 NZD/kg (6 USD/kg), which is comparable to the conventional practice of autoclaving followed by landfilling. The potential environmental impacts of this process were found to be negligible; meanwhile, this practice significantly reduced the use of limited landfill space.

- **Keywords:** Hydrothermal deconstruction; COVID-19; Process modelling; PPE; Wet oxidation

Zong Yang Kong, Gabriel Contreras Zarazúa, Hao-Yeh Lee, Justin Chua, Juan Gabriel Segovia-Hernández, Jaka Sunarso. *Design of novel side-stream hybrid reactive-extractive distillation for sustainable ternary separation of THF/ethanol/water using mixed entrainer*. Pages 574-588.

This work explored the possibility of using mixed entrainer in a hybrid reactive-extractive distillation to improve the sustainability of the recovery process for the ternary azeotropic mixture containing THF/ethanol/water. A double column reactive-extractive distillation (DCRED) using mixed entrainer (i.e. dimethyl sulfoxide (DMSO) + ethylene glycol (EG)) is initially proposed and intensified to a side-stream DCRED (SS-DCRED). Both the initial DCRED and SS-DCRED designs are optimised using particle swarm optimisation (PSO) to obtained optimum column configurations. The sustainability of the proposed processes using mixed entrainer are compared against pure EG as entrainer based on five different

indicators, i.e. economic, environmental, safety, operational controllability, and thermodynamic efficiency. Generally, it was demonstrated that using mixed entrainer provides significant improvement in all sustainability indicators. Although there may be some trade-offs in the controllability and economic, such drawbacks are consistent with previous publications where the improvement in sustainability are always achieved at an expense of an increase in the economics. Overall, it was revealed that the optimised SS-DCRED using mixed entrainer provides the best improvement to the economic, controllability, safety, environmental, and thermodynamic efficiency by 21 %, 97 %, 19 %, 29 %, and 100 %, with respect to using pure entrainer, which reflects the sustainability of the proposed process.

- **Keywords:** Hybrid reactive-extractive distillation; Ternary azeotropic separation; Energy-intensified techniques; Side-stream configuration; Mixed entrainer; Inherent safer design

Jiajia Xu, Lin Zhang, Yujun Liu, Qiangling Duan, Kaiqiang Jin, Qingsong Wang. *Electrochemical performance and thermal stability of 18650 lithium-ion battery with water mist after high-temperature impact*. Pages 589-599.

Exposure of LIB to high temperatures may cause certain damage or even fail to work. In this study, the electrochemical performance, the thermal stability and the critical heat of 18650 LIBs with/without water mist after high-temperature impact are experimental investigated. The results demonstrate that water mist raises the critical temperature of battery damage by about 40 °C. With increasing temperature, the electrochemical performance of the battery decreases, primarily caused by loss of lithium-ion. Moreover, water mist also improves the thermal stability of batteries after high-temperature impact, as demonstrated by the higher onset temperature of thermal runaway and activation barriers. Under the use of water mist, the critical heat that the battery performance is not affected and the critical heat for battery damage are obtained based on the increase and distribution of temperature and double integral, which are 2489.46 ± 47.7 J and 4777.63 ± 71.55 J, respectively. This work reveals that water mist could alleviate the damage to the battery caused by high-temperature impact, but when the heat exceeds the critical heat, the damage is irreversible. These findings could provide suggestions for the use of water mist in the thermal safety design of batteries in the future.

- **Keywords:** Lithium-ion battery; High-temperature impact; Water mist; Electrochemical performance; Thermal stability

Yasri, A.R. Laiju, V.R. Sankar Cheela, Abdoulaye Thiam, Yemane G. Asfaha, S. Kanmani, Edward (Ted) P.L. Roberts. *Emerging applications, reactor design and recent advances of electrocoagulation process*. Pages 600-616.

The ability of electrocoagulation (EC) to treat water and wastewater effectively is well-known. There are several improvements that have been adopted in EC processes to enhance treatability, performance, or reduce environmental impacts. Such improvements include: addition of air and hydrogen peroxide to generate radicals; use of an air cathode to reduce energy consumption; polarity reversal for reducing electrode passivation; and use of renewable energy generation as the source of electrical energy. Each of these improvements exploits different mechanisms to improve the applicability of EC. There are several emerging applications where EC has been shown to be suitable, including microplastics, nanoparticles, emerging contaminants, oil and grease, and disinfection.

- **Keywords:** Electrocoagulation; Emerging applications; Emerging contaminants; Water and wastewater treatment

Lu-Tao Zhao, Ting Yang, Rui Yan, Hong-Bo Zhao. *Anomaly detection of the blast furnace smelting process using an improved multivariate statistical process control model*. Pages 617-627.

Anomaly detection and early warning of the blast furnace ironmaking process is an important research direction of blast furnace production. In this paper, through the analysis and optimization of the multivariate statistical process control (MSPC) model, MSPC based on TOPSIS and the grey (GT-MSPC) model is established based on the problems of missing alarms, false alarms and untimely prediction in the abnormal detection process of the traditional blast furnace ironmaking production process. First, a composite volatility (CV) that consists of the squared prediction error and T2 is computed to form the MSPC model. The parameters of different training set sizes and different alarm conditions are optimized by using the technique for order preference by similarity to an ideal solution model to optimize the effect of anomaly detection and fault diagnosis. Second, according to the results of the contribution plot, the fault diagnosis of abnormal occurrence is carried out, the main influencing factors of abnormal occurrence are analysed, and the monitoring is strengthened. Finally, the grey model is used to predict CV to realize anomaly early warning and form the GT-MSPC model. By collecting the field data of blast furnace production and performing empirical analysis, the results show that the GT-MSPC model has higher anomaly detectability. The detection rate is 50 % higher than that of the manual observation method, and the GT-MSPC model alarms 16.4861 min earlier than manual detection method. Fault diagnosis can accurately locate the main influencing factors of blast furnace anomalies, such as the furnace body static pressure and differential pressure. In summary, the GT-MSPC model realizes the accurate identification and prediction of anomalies and greatly reduces the occurrence of missing and false alarms and untimely prediction in the blast furnace system, thus reducing the risk of blast furnaces. It can be used to assist field engineers in dealing with abnormal faults and improve the product quality and production safety of blast furnace ironmaking.

- **Keywords:** Blast furnace; Anomaly detection; Fault diagnosis; MSPC; Early warning

Jiandong Liu, Xinrong Fu, Rongfang Yuan, Zhongbing Chen, Beihai Zhou, Huilun Chen. *Carbon sources derived from corncobs enhanced nitrogen removal in SBBR treating low C/N domestic sewage*. Pages 628-637.

Domestic sewage has the characteristics of low carbon to nitrogen ratio (C/N), so an external carbon source is required to increase the denitrification performance of the system. Agricultural waste carbon sources have attracted much attention due to their wide range of sources and low cost. Therefore, this study investigated the corncob pretreated with acid and alkali as the external carbon source. Then the effect on nitrogen removal was further determined by sequencing batch biofilm reactor (SBBR). The results showed that the alkali pre-treated corncob had a higher carbon release capacity; the COD cumulative release amount was 123.5 mg/g·L within 16 days. It had an excellent denitrification rate, with a total nitrogen removal rate of 90.1%. In addition, the denitrification rate of alkali pre-treated corncob (100 g) as a carbon source was equivalent to that of sodium acetate (influent C/N ratio: 15). At this time, the total nitrogen removal rate reached a maximum of more than 90%. Microbial community analysis discovered that microbial abundance and diversity increased after adding corncob carbon sources. Among them, the contents of Firmicutes, Macellibacteroides, and Hydrogenophaga were significantly increased, which played a decisive role in degrading cellulose and using cellulose as a carbon source for denitrification. Besides, denitrifying bacteria such as Proteobacteria, Thauera, and Gemmatimonas were also abundantly aggregated, indicating that the denitrification in SBBR was enhanced. These findings collectively suggest that alkali pre-treatment of corncob as a carbon source could effectively improve the denitrification performance of low C/N ratio wastewater.

- **Keywords:** Carbon source; Corncob; Denitrification; Low C/N ratio wastewater

Jiashun Zhou, Zhihe Cao, Baozhong Ma, Yongqiang Chen, Chengyan Wang. *Effective separation and recovery of iron and chromium from laterite residue in the presence of calcium chloride*. Pages 638-648.

In nitric acid pressure leaching (NAPL) for the treatment of limonitic laterite ores, the comprehensive utilization of leach residue is significant for resource recovery and environmental protection. In this work, the recovery and separation of iron and chromium from NAPL residue by metallization reduction roasting−magnetic separation with calcium chloride as additive was studied. The following optimum parameters were obtained: 1100 °C roasting temperature, 25 % reductant dosage, 40 min roasting time, 7 % calcium chloride dosage, 200 mT magnetic field intensity, and 40 s rod mill time (D50 = 7.20 μm). Under these optimum conditions, 81 wt% iron content in the concentrate and 7.4 wt% chromium in the tailings were obtained. The corresponding recovery rates of iron and chromium were 95 % and 64 %, respectively. The microstructure and composition of leach residue and process products were investigated by SEM, EDS, and XRD to study the phase transition and polymerization of substances during roasting. The results showed that iron was mainly enriched in the magnetic concentrate, and chromite and silicate minerals dominated the tailings. Analysis of the action of calcium chloride in the reduction roasting revealed that calcium chloride was beneficial for the liberation of Fe from fayalite and the migration and polymerization of iron.

- **Keywords:** Calcium chloride; Nickel laterite; NAPL residue; Iron; Chromium

Linsheng Zhang, Jian Ruan, Zhiyan Lu, Zishuai Xu, Guanchao Lan, Jianlong Wang. *Thermal hazard assessment of 3-nitro-1,2,4-triazole-5-one (NTO) synthesis*. Pages 649-655.

In order to assess thermal hazard of 3-nitro-1,2,4-triazole-5-one (NTO) synthesis, the thermal decomposition behaviors of 1,2,4-triazole-5-one (TO), nitrification liquor and NTO under the kinetic and adiabatic environments were explored by virtue of differential scanning calorimeter (DSC) and accelerating rate calorimeter (ARC). The outcomes provide key safety parameters for the safety of NTO during the reaction process, transportation and preservation. In addition, the exothermic characteristics of TO nitrification process was monitored by automatic multifunctional reaction calorimeter (EasyMax HFCal), the total heat release of nitrification reaction at different feeding temperatures were comparatively studied and the relationship between feeding rate and thermal runaway in NTO synthesis process is explored. The outcomes reveal that the thermal release rate is high at the reactive feeding phase, and the feeding rate ought to be regulated. The thermal variables such as adiabatic temperature elevation (ΔTad) and maximal temperature of the synthesis reaction (MTSR) were calculated to evaluate the thermal hazard of NTO synthesis at diverse feeding temperatures. To ensure the safety of NTO industrial production, these studies provide theoretical basis and guidance for controlling the thermal runaway risk of NTO synthesis.

- **Keywords:** 3-nitro-1,2,4-triazole-5-one; Nitration; Reaction calorimeter; Cooling failure; Thermal hazards

Yasaman Davarikia, Abdolreza Aroujalian, Parisa Salimi. *Immobilization of TiO2 nanoparticles on PES substrate via dopamine and poly (vinyl alcohol) for long-term oil/water purification*. Pages 656-668.

In this paper, a facile procedure is presented to prepare a membrane with antifouling properties based on Tio2 and polyvinyl alcohol hydrophilicity and the high adhesion of

dopamine. First, vapor-induced phase separation was used to prepare the PES substrate, and then TiO2 nanoparticles were anchored on the membrane surface with the assistance of dopamine and PVA. The nanoparticles were uniformly immobilized on membrane surface, significantly advancing the performance of the PES membrane. Results of contact angle measurements revealed an outstanding improvement in the surface hydrophilicity. The fabricated membranes had higher water permeation during oil/water separation and also greater oil rejection with approximately 50% improvement compared with the pristine membrane. Moreover, a FRR of 81% after fouling with oil droplets, increasing in subsequent cycles to 87%, showing a good regeneration capability during long-term performance was achieved by the modified membrane, which confirms the low fouling tendency. Stability of NPs was investigated through a cross-flow water flux, followed by weight measurements, FE-SEM and EDX analysis prior and after the flux. The results proved the stability of modifiers on the membrane surface.

- **Keywords:** Surface modification; Oil/water separation; Long-term performance; Antifouling; Stability; TiO2

Lin Liu, Xiaohang Xu, Jialiang Han, Jian-Ming Zhu, Shenghao Li, Longchao Liang, Pan Wu, Qixin Wu, Guangle Qiu. *Heavy metal(loid)s in agricultural soils in the world's largest barium-mining area: Pollution characteristics, source apportionment, and health risks using PMF model and Cd isotopes*. Pages 669-681.

Barium (Ba) mining and smelting activities release heavy metal(loid)s (HMs) that may cause threats to agroecological systems and human health. Here, contamination features, source apportionments, and associated health risks from agricultural soils were systematically investigated. According to descriptive statistics and HM single-pollutant indices, Ba, Cd, and As are priority control pollutants. Spatial interpolation and autocorrelation results indicate that Ba, Cd, and Zn have an aggregated distribution, clustered in the northwest of the study area in Guizhou Province, SW China. Pollution sources were apportioned based on multivariate statistics and a positive matrix factorization (PMF) model. As Cd is the dominant pollutant in Ba mines, Cd isotopic fingerprints and Bayesian isotopic mixing models in R were used to characterize the sources of Cd. PMF source apportionment and Bayesian isotopic mixing modeling indicate that the predominant sources of Cd in agricultural soils in Ba mining areas are mining and smelting, followed by agricultural activities and atmospheric deposition. PMF source apportionment suggests that the primary sources of HMs are Ba mining/smelting and agriculture, followed by sewage irrigation, and atmospheric deposition. Barium, As, and Cd pose the highest non-carcinogenic and carcinogenic risks, and should be prioritized for control.

- **Keywords:** Heavy metal(loid)s; Barium mining; Positive matrix factorization; Cd isotope; Exposure risks

J.B. Liyanage, P.G. Ranjith, W.G.P. Kumari. *A study of the short-term leaching behaviour of a modified expansive cement in groundwater for mining and mineral extraction*. Pages 682-692.

The modified expansive cement, Slow Releasing Energy Material Agent (SREMA), has been introduced as a greener alternative to conventional mining. SREMA is similar to Ordinary Portland Cement (OPC) in its constituents, containing mostly CaO, and Al2O3, SiO2, MgO, Fe2O3, CaSO4 in minute amounts, but including Soundless Chemical Demolition Agents (SCDAs) as the base material. SREMA is an effective method of mining without causing severe environmental damages by undergoing expansion when injected to a borehole, causing fractures in the surrounding materials and exposing the fossil fuel, metals, minerals or ores of interest that may lie within. Nonetheless, its leaching

behaviour in underground water conditions has not been explored to date. The aim of this study is to investigate the leaching behaviour of SREMA in typical geological conditions using a serial batch leaching method and propose mitigation techniques to minimise the leaching effect leading to contamination of water. According to the experimental results, calcium leaching is much more prominent than that of other cations present in the solid matrix. When compared with the OPC, the calcium leaching behaviour of both hydrated and hydrating SREMA is comparably higher in all considered leachants, due to the larger mass percentage of CaO and high porosity of SREMA. Overall, hydrated SREMA shows the greatest calcium leaching of 835 ppm in 7 days under saline conditions of 5 wt% NaCl, which is over twice the leaching seen in the presence of water. A similar tendency is seen with hydrating SREMA as well but with a maximum leaching of 539 ppm. An increase in calcium leaching is observed, with over a 2-fold rise in leaching compared to that in water, as the basic pH reduces, with the formation of globular katoite. Moderated calcium leaching is seen under acidic conditions, even though the basic nature of Ca(OH)2 would suggest otherwise. The saturation indices (SIs) and degree of calcium leaching have been calculated to understand the behaviour of solubility in the presence of the considered leachants. In addition, potential modifications are proposed to improve the composition of SREMA to reduce the leaching effects revealed by experimentation, while maintaining its expansive qualities.

- **Keywords:** Slow releasing energy material agent (SREMA); Soundless chemical demolition agent (SCDA); Expansive cements; Ordinary portland cement (OPC); Leaching; Water quality; Mining

Yasunori Kikuchi, Noriko Torizaki, Leena Tähkämö, Annamari Enström, Sari Kuusisto. *Life cycle greenhouse gas emissions of biomass- and waste-derived hydrocarbons considering uncertainties in available feedstocks*. Pages 693-703.

Sustainable chemical production requires renewable feedstocks. Biomass- and waste-derived production is a method for producing chemical products from renewables. In this study, we explore sustainable chemical production applying renewable feedstocks crude palm oil, rapeseed oil, palm fatty acid distillate, used cooking oil, inedible animal fat, inedible fish fat, and algae oil. Hydrotreated vegetable oil has been applied as the raw material for cracking on petrochemical sites and conversion into chemicals based on existing technology patents. A life cycle assessment was used to examine whether this production route can support a reduction in nonbiogenic greenhouse gas (GHG) emission by the production and use of renewable-derived hydrocarbons (RDHC) as the functional unit (FU). The life cycle GHG of the FU ranged between 2.87 and 3.29 kg-CO2eq/FU for three types of feedstock mix, considering their availability and RDHC production capacity, whereas that of fossil-based life cycle is 4.59 kg-CO2eq/FU. Due to the limited availability and wide range of needs, the sourcing of renewable feedstocks could become competitive in the near future. The development and implementation of technologies applying various resources as feedstocks for chemical production are strongly needed toward a carbon-neutral chemical production.

- **Keywords:** Life cycle assessment; Sustainability; Hydrotreated vegetable oil; Attainable region; Emerging technology; Proof of concept

Maryam Afsharpour, HamidReza Behtooei, Marzieh Shakiba, Vicenç Martí, Shahriar Salemi Parizi. *Novel N,P,S co-doped graphenic SiC layers (g-SiC) in visible-light photodegradation of antibiotics and inactivating the bacteria*. Pages 704-717.

In this work, the green synthesis of N, P, S-doped graphenic silicon carbide (g-SiCs) and their potential application as the high performance photocatalysts for the removal of

antibiotics (Tetracycline (TCL), ciprofloxacin (CIP), and Amoxicillin (AMX)) and bacteria (S. aureus and E. coli) was investigated under visible light. Synthesized g-SiCs show excellent potential in the removal of organic pollutants compared to commercial SiC. These results are obtained due to the graphenic structure of synthesized g-SiC which increases the electron transfer and reduces the rate of electron-hole recombination. Also, the positive charged Si atoms in the g-SiC structure enhance the adsorption of oxygen molecules to produce the oxygenated radicals which are active species in the degradation of organic pollutants. To improve the photocatalytic activity, nitrogen, phosphor, and sulfur were doped onto the g-SiC structure. The resulting doped catalysts the enhanced photocatalytic activities compared to corresponding non-doped g-SiC. The enhanced photocatalytic activity of doped g-SiC structures could be explained in terms of higher surface area, more defects for better absorption, lower band gap, and more positive charge in Si atoms to the better formation of oxygenated radicals for degradation of antibiotics. This work also introduces these new metal-free materials for photocatalytic inactivating bacteria via the produced active radicals.

- **Keywords:** G-SiC; Doped; Metal-free; Photocatalyst; Antibiotic; Bacteria