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Ahmed Zohair Djeddi, Ahmed Hafaifa, Nadji Hadroug, Abdelhamid Iratni. *Gas turbine availability improvement based on long short-term memory networks using deep learning of their failures data analysis*. Pages 1-25.

Practically, a maintenance operation is performed on industrial equipment after scheduled planning that depends on the average useful life of this equipment (Mean Time Between Failures or Mean Time to Failure). Hence, in the industry, the use and the processing of data certainly improve productivity. But they induce a complexity of the industrial system caused by the different misconduct and measurements. This requires significant expenses on the safety, reliability, and availability of this type of machine. In this work, a new approach is proposed to determine the degradation indicators of a GE MS 5002B gas turbine installed on the Hassi R'Mel gas field in southern Algeria. The proposed approach is based primarily on Long Short-Term Memory LSTM networks, using in-depth learning of operating data. We are starting with the study of their reliability and their prognosis to validate and improve their performance, by optimizing their life cycle costs through good operating, repair, and maintenance planning. The objective is to remedy the problems mentioned by the processing of conventional data and predict their evolution and progression during the lifetime of the examined turbine. By combining actual reliability tests with predictions based on their failure rates to ensure good operating safety, and availability of the turbine system by controlling aging and degradation indices with satisfaction in environment and yield of this rotating machine.

- **Keywords:** Failures' analysis; Failures prediction; Deep learning; Availability; Reliability distribution; Degradation indicators; Prognosis; Long Short-Term Memory networks; Gas turbine

Gongduan Fan, Shulei Bao, Yang Guo, Mingqian Xia, Mingcai Lin, Shujuan Cai, Weifang Ruan, Tingting Liao, Zhongsen Yan. *Spatio-temporal variations of salinity and analysis of desalination factors in a Chinese coastal storage reservoir*. Pages 26-35.

Coastal reservoirs could be used to store freshwater in coastal cities, but the conversion of coastal reservoirs to freshwater reservoirs is relatively time-consuming, and coastal reservoirs are facing a risk of salinization. Taking Zhuyu Lake as the research object, the Spatio-temporal variations of water salinity under different seasons were investigated using the field survey and modeling. The influencing factors of the water salinity of the reservoir were analyzed to discover the variation mechanism. The results showed that the disturbance of overlying water is the most significant factor affecting the salt release

of sediment, and salt release was increased by 63.3% with the disturbance. The depth of the overlying water and the salt content of bottom sediment also significantly affected the release of salt, with maximum enhancement by 23.1% and 45.6%, respectively. The microbial content in the bottom mud played an essential role in maintaining the salt, and inhibiting the microbial activity could enhance the release of salt by 35.7%. Therefore, disturbing the sediment by using disturbance ships or aeration devices, and the establishment of a long-term periodic plant harvesting belt could be used in the coastal fresh reservoirs desalination and slowing down the salinization of fresh reservoirs.

- **Keywords:** Salinity; Spatio-temporal variations; Coastal storage reservoir; Desalination factors

Longjie Liu, Qingping Wang, Jiajiang Lin, Gary Owens, Zuliang Chen. *Enhanced 17α-estradiol removal by biosynthesized rGO@Fe NPs using a response surface methodology*. Pages 53-60.

Recently, estrogen has attracted widespread concern because it is increasing being detected in wastewater treatment plants. While techniques for estrogen removal have been reported, these have mostly focused on exploring the effect on removal using simple single-factor experiments, rather than applying more complex multifactor mathematical models to wastewater treatment. In this study, reduced graphene oxide-based iron nanoparticles (rGO@Fe NPs) were used for 17α-estradiol (αE2) removal based on adsorption and Fenton oxidation. A response surface methodology, based on a Box-Behnken design, was used to determine the relationships between critical operation factors (pH, temperature, αE2 concentration, rGO@Fe NPs dose and H2O2 concentration) and removal efficiency to establish the optimal conditions for 1 mg L−1 αE2 removal. Under the determined optimal reaction condition of pH 6.0, temperature 40 °C, 0.08 g L−1 rGO@Fe NPs dose and 6 mM H2O2, a maximum removal efficiency of 99.9% was obtained. Subsequently, the presence of co-existing anions (Cl−, SO42− and NO3−) significantly decreased the removal efficiency of αE2. However, αE2 removal from domestic wastewater could be increased by 38.0% when applying RSM results. Moreover, αE2 removal by rGO@Fe NPs remained stable over five reuse cycles indicating that rGO@Fe NPs would be an efficient and practical advanced materials for αE2 removal.

- **Keywords:** 17α-estradiol; Biosynthesis; Reduced graphene oxide; Iron nanoparticle; Response surface methodology

Federico Ustolin, Ilias C. Tolias, Stella G. Giannissi, Alexandros G. Venetsanos, Nicola Paltrinieri. *A CFD analysis of liquefied gas vessel explosions*. Pages 61-75.

Hydrogen is one of the most suitable candidates in replacing fossil fuels. However, storage issues due to its very low density under ambient conditions are encountered in many applications. The liquefaction process can overcome such issues by increasing hydrogen's density and thus enhancing its storage capacity. A boiling liquid expanding vapour explosion (BLEVE) is a phenomenon in liquefied gas storage systems. It is a physical explosion that might occur after the catastrophic rupture of a vessel containing a liquid with a temperature above its boiling point at atmospheric pressure. Even though it is an atypical accident scenario (low probability), it should be always considered due to its high yield consequences. For all the above-mentioned reasons, the BLEVE phenomenon for liquid hydrogen (LH2) vessels was studied using the CFD methodology. Firstly, the CFD model was validated against a well-documented CO2 BLEVE experiment. Secondly, hydrogen BLEVE cases were simulated based on tests that were conducted in the 1990s on LH2 tanks designed for automotive purposes. The parametric CFD analysis examined different filling degrees, initial pressures and temperatures of the tank content with the aim of comprehending to what extent the initial conditions influence the blast

wave. Good agreement was shown between the simulation outcomes and the LH2 bursting scenario tests results.

- **Keywords:** Liquid hydrogen; Safety; Physical explosion; CFD analysis; Liquid CO2; Risk assessment

Mina Aghaei, Kamyar Yaghmaeian, Mohammad Sadegh Hassanvand, Masud Yunesian, Ramin Nabizadeh, Fatemeh Yousefian, Mahdi Hosseini Beinabaj, Mohammad Hossein Hedayati. *Spatial and temporal variation of endotoxin concentrations at composting facilities in one of the largest solid waste management facilities in the Middle East*. Pages 76-83.

Composting activities at open-air facilities can be a source of contaminants including bioaerosols. Exposure to bioaerosols and their constituents can have a potential impact on those involved in waste management and those living in the vicinity of such facilities. This study aims to investigate the temporal and spatial variation in endotoxin concentrations as a biohazard at waste composting facilities in one of the largest municipal solid waste management complexes in the Middle East. The total suspended solids (TSP) and airborne endotoxin were collected by the active method using a pump with an airflow rate of 2 L/min, and 37-mm glass fiber filters. TSP was determined by gravimetry, and then extraction was done in pyrogen-free containers by adding 0.05% Tween 20 in 10 ml of PFW (Pyrogen Free Water), and the endotoxin concentration was determined by the Limulus amebocyte lysate (LAL) method. The results showed high concentrations of endotoxins in composting processes. The highest mean concentrations of ambient air TSP were found in granulation sites (2937 µg/m3) and preprocessing halls (998 µg/m3) and the lowest in the windrow sites (302 µg/m3). The average concentration of endotoxin in the ambient air of granulation, pre-processing and post-processing sites were 48.3, 17.8, and 10.6 times the mean concentrations in the windrow sites, respectively. A significant difference was found in endotoxin and TSP levels between five locations ($P = 0.001$ and 0.008 respectively), and spatial variation was observed in this study. A good correlation was observed between reported endotoxin concentration and airborne dust ($r = 0.797$) in composting plant. The evidence provided by this study will help the operators of facilities to be aware of the pollution of different locations involved in composting, and regulators to focus on improving risk assessments at these facilities and also take precautions where a high level of contaminants is reported.

- **Keywords:** Endotoxin; Variation; Composting; Solid waste management

Xu Diao, Juncheng Jiang, Lei Ni, Ahmed Mebarki, Guodong Shen. *Electrification hazard of turbulent pipe flow: Theoretical approach and numerical simulation*. Pages 84-95.

The present paper deals with electrostatic characteristics, i.e., space charge density and electrostatic potential under turbulent flow in pipes with and without leakage. This paper considers the charge conservation equation and proposes theoretical models able to calculate the space charge density of intact and leak pipes. The distributions of the space charge density and electrostatic potential are investigated through numerical simulation. For the case study used for validation purposes, the space charge density obtained by numerical simulations is compared with the experimental results. The results show that the proposed model is capable of calculating adequately the distribution of the space charge density in pipes. The effects of flow velocity and pipe diameter on the electrostatic characteristics of intact and leak pipes are then investigated. The results show that, for intact pipes, the maximum electrostatic potential appears in the central area of the pipe and increases slowly with the increase of the velocity, while the maximum potential decreases with the increase of the pipe diameter. For leak pipes, the maximum potential

takes place at the leak aperture, and increases with the increase of flow velocity and pipe diameter. In order to reduce the possibility of electrostatic discharge, the flow velocity ought to be controlled below 2.5 m/s, and the pipes with smaller diameter shall be used as far as possible when meeting the requirement for use.

- **Keywords:** Flow electrification models; Numerical simulation; Space charge density; Electrostatic potential; Leak pipe

Yuto Mizuta, Motohiko Sumino, Hiroaki Nakata, Yuichiro Izato, Atsumi Miyake. *Analysis of pressure behavior during runaway reaction with case studies of various depressurization designs*. Pages 96-105.

In chemical plants, safety valves are installed on process equipment where pressure rise would occur to prevent their rupture. However, it is difficult to estimate accurate vent size for two-phase flow, and the analysis of pressure rise behavior during a runaway reaction is important. However, ISO method sometimes gives unpractical vent size, therefore, a detailed process dynamic simulation model was constructed in this study. A detailed model was constructed with Aspen and Advanced Reactive System Screening Tool (ARSST) experimental data. The model for depressurization from reactor was the refined omega-method of ISO, which was programmed with Aspen Custom Modeler. The case studies of dynamic simulation are carried out and the result of vent size estimated from ISO method were compared. In addition, some case studies on various process conditions and safety valves such as diameters and set pressures of safety valve, the presence of exhaust gas lines and different solvents were carried out. Different combinations of these conditions produced significantly different behavior in the runaway reaction. Therefore, these results lead to the understanding of runaway reaction and may expect to provide some options for constructing safer processes practicably and economically.

- **Keywords:** Runaway reaction; Vent sizing; Two-phase flow; Dynamic simulation; Liquid decrease; Exhaust gas line

Mohsin Pasha, Hong Zhang, Minjing Shang, Guangxiao Li, Yuanhai Su. *CO2 absorption with diamine functionalized deep eutectic solvents in microstructured reactors*. Pages 106-119.

Deep eutectic solvents (DESs) have gained much attention to capture CO2 nowadays because of their simpler synthesis, higher sustainability and better eco-friendly properties compared to ionic liquids and conventional amine sorbents. Herein, we analyzed the CO2 absorption performance of five novel diamine functionalized DESs in microstructured reactors (MSRs) with metal foams as packing materials. Interestingly, the DES functionalized with N-methyl-1,3-propanediamaine (MAPA) showed remarkable absorption performance without significant viscosity rise. The CO2 loading and absorption efficiency of this DES could reach 0.78 mol of CO2 / mol of diamine and 98% at the gas to liquid flow rate ratios of 640 and 240, respectively. Even computational studies showed that the ethylenediamine (EDA) functionalized DES had the highest CO2 uptake ability due to the low energy barrier, but sudden rise in viscosity of the EDA functionalized DES reduced its CO2 absorption ability compared to the MAPA functionalized DES. Further experiments indicated that the MAPA functionalized DES showed low heat of absorption and remarkable regeneration ability. Overall rate constant and absorption flux of this DES were higher than most previously used amine functionalized DESs. Consequently, the unification of this remarkable DES and microreactors has great process intensification potential for CO2 absorption.

- **Keywords:** CO2 capture; MAPA functionalized DES; Viscosity; Microstructured reactor; Process intensification

Iman El Gheriany, Mohamed Helmy Abdel-Aziz, El-Sayed Zakaria El-Ashtoukhy, Gomaa H. Sedahmed. *Electrochemical removal of urea from wastewater by anodic oxidation using a new cell design: An experimental and modeling study*. Pages 133-145.

Chlorine-mediated electrochemical urea oxidation was investigated using a new electrochemical cell design with horizontally oriented electrodes. By virtue of the novel electrode configuration, the new electrochemical cell is self-stirred by the H2 bubbles evolving at the cathode surface and contains a built-in cooler to remove excess heat generated during electrolysis. The effect of current density, pH, NaCl concentration and initial urea concentration on the urea removal and specific electrical energy consumption were investigated. The % urea removal ranged from 55% to 90% depending on the operating conditions. The rate of urea removal increased with increasing current density and NaCl concentration, while increasing the solution pH and initial urea concentration were found to decrease the rate of removal. Energy consumption decreased with increasing NaCl concentration and increasing initial urea concentration. A kinetic approach and response surface methodology were used to model the temporal profile of urea oxidation and to optimize the process variables. After 33.4 min of electrolysis of a solution containing 348.6 ppm urea, 3% NaCl concentration and an initial pH of 5.6 using an applied current density of 4.6 mA/cm2 (2.6 A), 73.8% urea removal could be achieved with an extremely low energy consumption of 9.58 kW hkg urea. The influential priorities of the five operating parameters on % urea removal and specific energy consumption were different. The obtained results revealed that the use of kinetic and statistical modeling is an adequate approach to optimize the process variables of electrochemical urea degradation.

- **Keywords:** Urea fertilizer; Wastewater; Electrochemical urea oxidation; Chlorine-mediated anodic oxidation; Agricultural runoff water; Artificial kidney

Ze Zhang, Shuting Zhang. *A new method of coal fine particles humidification and agglomeration: Synergistic dust suppression with composition of soap solution*. Pages 146-156.

Coking plants usually use surfactants to increase the surface wettability of fine coking coal particles, promote its agglomeration, and achieve the purpose of reducing dust emission. The Soap solution as a chemical agent contains not only soap base active ingredients, but also abundant surfactants and antifouling redeposition agents. The aim of this study is to optimize the dust suppression effect by blending the chemical composition proportion of existing soap solution, and analyze the interaction mechanism of each component on the surface of fine particles, then realize the dust suppression with low cost and high dust suppressor effect. Keeping the other ingredients remain the same, the hydrophilic organosilicone and carboxymethyl starch were selected as antifouling redeposition agents; the anionic surfactant sodium fatty acid methyl ester sulfonate (MES), non-ionic surfactant fatty acid methyl ester ethoxide (FMEE) and fatty alcohol polyoxyethylene ether (AEO-9) were used to mix in different proportions. The wetting effect and adsorption rate of the compound soap solution on the surface coal were tested. Then the particle coating efficiency, size growth rate and dust removal amount during the spraying of compound soap solution were tested and mechanism analysis in the device developed by the laboratory. The result indicates the wettability and agglomeration efficiency of coal particles can be obviously improved by increasing the proportion of FMEE and AEO-9. Compared with carboxymethyl starch, using hydrophilic organosilicon as antifouling redeposition agent can increase the adsorption capacity of raw coal to surfactants by 5% and the particle growth rate by 2%.

- **Keywords:** Coking coal; Redeposition agent; Surfactant; Wettability; Agglomeration

Jun Zhou, Haonan Zhang, Tong Zuo, Qinwei Jia, Luyu Wang, Yaqi Tian, Lei Gong, Ying Zhou, Jin Wang. *Enhanced copper-containing wastewater treatment with MnO2/CNTs modified anode microbial fuel cell*. Pages 157-167.

A microbial fuel cell (MFC) was constructed with CNTs, 0.02gMnO2/CNTs and 0.03gMnO2/CNTs modified graphite anode prepared by coating for enhancing copper wastewater treatment. The SEM, XRD and FTIR results showed that MnO2/CNTs and CNTs were successfully attached to the graphite electrode, indicating that the electrode was modified successfully. The surface wettability test showed that the decrease of the contact angle of the modified anode led to the increase of hydrophilicity, which was more conducive to microbial adhesion. The surface contact angle of CNTs modified electrode was the smallest, which was 11.17°. The maximum output voltage, power density and copper removal rate of 0.03gMnO2/CNTs modified anode MFC were 0.67 V, 1044.21 mW/m2 and 98.93% respectively, which were 52.3%, 466.3% and 50.5% higher than those of unmodified anode. XPS results showed that the reduction products were Cu2O and Cu. Meanwhile , high throughput sequencing showed that CNTs and MnO2 could improve the richness and diversity of microbial community. MnO2/CNTs modified-anode accelerated the enrichment of electro-active bacteria such as Proteobacteria, Firmicutes and Bacteroidetes.

- **Keywords:** MFC; Microorganism; Modified electrode; Copper wastewater

Yan Bao, Lu Gao, Feitong Wang, Jianzhong Ma. *Heterocyclic cationic Gemini surfactants for efficient antibacterial, dispersion and fixation*. Pages 168-177.

Gemini surfactants are highly demanded worldwide due to their promising applications in paper, medical hygiene, and textile. However, the design of Gemini surfactant integrated with biosafety and multi-functionality has been considered a long-standing demand for environmental protection and industry cost. Hence, three kinds of heterocyclic cationic Gemini surfactants (C12-2 P-C12, PC4H5N, C4H9NO, C3H4N2) with different hydrophilic groups were synthesized and employed to enhance antibacterial, dispersion, and fixation in leather processing. Their surface activity was measured by a series of analytical and testing methods, including the surface tension (γcmc), wettability and emulsifying ability. The results showed that the surface activity of the Gemini surfactants were followed the order of C12-2 C4H5N-C12 (γcmc=28.65 mN/m)< C12-2 C4H9NO-C12 (γcmc=25.85 mN/m)< C12-2 C3H4N2-C12 (γcmc=23.31 mN/m). Their antibacterial activities were assessed by means of Staphylococcus aureus. C12-2 C3H4N2-C12 obtained a superior antibacterial rate (~100%) owing to its high charge density. And compared with the traditional soaking programs (JFC and commercial fungicides), the sheepskins treated by C12-2 P-C12 exhibited favorable antibacterial properties and fiber dispersion. Among them, the protein content in the soaking solution containing C12-2 C3H4N2-C12 increased notably by 68.0 μg/mL in contrast to the traditional soaking solution (23.8 μg/mL), indicating that C12-2 C3H4N2-C12 has the best effect for fiber dispersion. For dyeing processing, the color fastness of the sheepskin treated by C12-2 C3H4N2-C12 could be improved from level 4 to level 4–5 compared to the commercial dye-fixing agent. And it led to significant changes of the dye concentration in waste liquid (from 1.1 g/L for comprasion to 0.1 g/L for C12-2 C3H4N2-C12), which may be imposed on the possibilities of the sustainable development of leather processing.

- **Keywords:** Gemini surfactant; Hydrophilic group; Fixing

Khalid A. Alamry, Ruby Aslam, Ajahar Khan, Mahmoud A. Hussein, Nada Y. Tashkandi. Evaluation of corrosion inhibition performance of thiazolidine-2,4-diones and its amino derivative: Gravimetric,

electrochemical, spectroscopic, and surface morphological studies. Pages 178-197.

To produce effective, less expensive molecules with minimum impact on the environment, the study aims to develop green corrosion inhibitors, which can significantly protect mild steel during its pickling and descaling treatment. Therefore, the present study describes the corrosion inhibition performance of two thiazole derivatives, namely thiazolidine-2,4-diones and its amino derivative 2-aminothiazolidin-4-one designated as TZD, and AT, respectively mild steel in 5%HCl solution through gravimetric measurement, electrochemical measurement (open circuit potential, electrochemical Impedance Spectroscopy, and potentiodynamic polarization). The spectroscopic measurement like FT-IR, UV–vis, X-ray photoelectron spectroscopy (XPS) along with surface morphological analysis like scanning electron microscopy-energy dispersive spectroscopy (SEM-EDS) and atomic force microscopy (AFM) was also carried out. Gravimetric studies suggested that the inhibitory effects of the proposed compounds improves with an increase in the concentration of TZD and AT and solution temperature, having the most significant efficiencies of 98.0% and 99.7%, respectively, at 5 × 10−4 M at 60 °C. According to electrochemical tests, the analyzed inhibitor molecules function as mixed-type corrosion inhibitors and improve corrosion charge transfer resistance. AFM, SEM, and EDS investigations indicated that TZD and AT molecules adhere and construct a surface protective layer.

- **Keywords:** Acid corrosion; Green inhibitor; Inhibition mechanism; AFM; XPS

Abu Reza M. Rashid, Muhammed A. Bhuiyan, Biplob Pramanik, Niranjali Jayasuriya. *A comparison of environmental impacts between rainwater harvesting and rain garden scenarios*. Pages 198-212.

Rain garden (RG) is a simple alternative to reduce pollutant loads carried through runoff. However, RG construction impacts the environment, where it demands evidence of net benefits generated once commissioned for operation. This study has simulated the reduction of runoff and pollutant loads due to the installation of RGs. Consequently, the reduction of the impacts on the environment was estimated using the LCA method. A comparison was carried out between the scenarios with and without RG with the most feasible (environmentally) rainwater harvesting (RWH) system. Three RG sizes are considered, such as 3, 4, and 6 m2 in dry, average, and wet annual rainfall conditions. The catchment-scale results showed that the runoff generation impacts of the RGs' operation phase were about (24–54%), (21–49%), (21–47%), and (14–45%) of the system without RG on eutrophication, human toxicity-carcinogenic, ecotoxicity-freshwater, and ecotoxicity-marine, respectively. However, once fabrication & installation were added, RG had much higher net impacts than without RG, except for eutrophication and ecotoxicity-freshwater. Hence, the net ecotoxicity-freshwater impact was lower for all scenarios except 4 and 6 m2 RG sizes during dry rainfall conditions. The most feasible RWH scenarios (e.g., 2000 & 3000 L tanks) had net impacts of 3–81% of the RG systems on global warming, human toxicity-carcinogenic, and ecotoxicity-terrestrial categories. On the other hand, RWH had net impacts of 105–200% on ozone depletion and eutrophication and 51–119% on the ecotoxicity-freshwater and ecotoxicity-marine of the RG systems.

- **Keywords:** Rain garden (RG); Rainwater harvesting (RWH); Global warming potential (GWP); Eutrophication, Life cycle analysis (LCA); Pollutant reduction

Wei Li, Xuesen Du, Zhi Li, Yaqin Tao, Jingyu Xue, Yanrong Chen, Zhongqing Yang, Jingyu Ran, Vladislav Rac, Vesna Rakić. *Electrothermal alloy embedded V2O5-WO3/TiO2 catalyst for NH3-SCR with promising wide operating temperature window*. Pages 213-220.

Vanadia-based catalysts are widely used in selective catalytic reduction (SCR) reaction for reducing nitrogen oxides emissions, however, they only exhibit sufficient DeNOx efficiency within a narrow temperature window. In this study, a catalyst embedded with electrothermal alloy was prepared. The catalyst surface temperature could be heated using the electrothermal alloy, in order to widen the operating temperature window of the V2O5-WO3/TiO2 catalyst. Experimental results revealed that the electrothermal alloy embedded V2O5-WO3/TiO2 catalyst can maintain superior NH3-SCR performance and high resistance to H2O in a wide gas temperature range of 100–400 °C by controlling the surface temperature. In the meantime, the NH4HSO4 poisoned catalyst could be efficiently regenerated through electric heating, and NOx conversion can be restored to the level of fresh samples. Additionally, the effect of additives including methylcellulose and glass fiber, on the physicochemical properties of the plate-type catalyst was also investigated, and the catalyst samples were characterized by means of BET, XRD, NH3-TPD, H2-TPR, TG and SEM-EDS. This study proves the electric heating strategy is a promising way to enhance the performance of the V2O5-WO3/TiO2 during wide temperature SCR applications.

- **Keywords:** SCR; Electrothermal alloy; Wide temperature range; Regeneration

Xiaohui Mei, Qing Zhao, Yi Min, Chengjun Liu, Henrik Saxén, Ron Zevenhoven. *Phase transition and dissolution behavior of Ca/Mg-bearing silicates of steel slag in acidic solutions for integration with carbon sequestration*. Pages 221-231.

Steel slag (SS) and carbon dioxide are two major waste products of the iron- and steelmaking process. Indirect aqueous carbonation of SS using Ca/Mg is a promising way for carbon capture, utilization, and storage (CCUS). However, it is generally accepted that the Si-rich layer produced during the leaching of silicates in SS has serious implications for the Ca/Mg recovery. Therefore, understanding the phase transition and dissolution behavior of Ca/Mg-bearing silicates of SS in acidic solutions is of vital importance for SS-based CCUS. In this work, three synthetic Ca/Mg-bearing silicates (Ca3MgSi2O8, Ca2MgSi2O7, and γ-Ca2SiO4) of SS were prepared and studied by leaching tests. Experiments were carried out with leaching silicate powder in 0.1 mol· L−1 HCl solution for various reaction time at room temperature. Results show γ-Ca2SiO4 and Ca3MgSi2O8 dissolved rapidly during the early leaching stages, giving more silica gel towards the end. Phases of Ca3MgSi2O8 and Ca2MgSi2O7 dissolved to yield Ca2+ and Mg2+ in solution in a similar ratio as in the original mineral. The Ca2MgSi2O7 phase was transformed into diopside (CaMgSi2O6) and silica gel during the acid leaching. Thus, the difference in phase transition of the studied Ca/Mg-bearing silicates is primarily related to the dissolution of the Si group in the crystal.

- **Keywords:** Steel slag; Ca/Mg-bearing silicate; Indirect aqueous carbonation; CO2 sequestration; Phase transition

Jian Chen, Dongsheng Wang, Liping Guo, Zhenghui Wang, Depeng Kong. *Experimental study on flame morphology and flame radiation of pool fire sheltered by plate obstacle*. Pages 243-250.

Liquid pool fires may represent the initiating fire hazard in many risk assessments associated with industrial plants. As real industrial fire scenarios generally include numerous obstructions, a pool fire burning behind an obstruction is a challenging task in the industrial risk assessment. A systematic investigation was conducted on the flame characteristics of a pool fire sheltered by a plate obstacle with different heights and geometrical dimensions, where the flame morphology, flame height, flame width and flame radiation flux were recorded and studied. The results show that the flame morphology for a pool fire sheltered by a plate obstacle can be divided in three types. For

the radiation heat flux evolution over the entire burning process, it was found that the plate obstacle above the fuel pool would lead to a larger peak value of the radiation heat flux. Using a physical and dimensionless method, prediction models for flame characteristics including flame width, flame height and maximum value of radiation heat flux were proposed.

- **Keywords:** Pool fire; Plate obstacle; Flame morphology; Flame radiation

Hui You, Ran Gao, Pengfei Hu, Ke Liang, Xiaorong Zhou, Xiaodong Huang, Mingzhang Pan. *Sensitivity analysis of diesel particulate filters to geometric parameters during soot loading and its multi-objective optimization*. Pages 251-265.

In order to improve the overall performance of diesel particulate filter (DPF) in the soot capture process, a multi-objective optimization model is developed based on the objective functions of maximum pressure drop and initial filtration efficiency. Firstly, the sensitivity analysis of the structural parameters of DPF are performed. Then the response surface model based on Box-Behnken is constructed, and diagnostic analysis and analysis of variance (ANOVA) are carried out for each response. Finally, the non-dominated sorting genetic algorithm-II (NSGA-II) is used to obtain the Pareto optimal solution. The research results show that the sensitivity of filter diameter to maximum pressure drop and initial filtration efficiency is higher than other parameters. The multi-objective optimization results are verified by GT-SUITE software, and the maximum relative errors of maximum pressure drop and initial filtration efficiency between the simulation and optimization results are 1.41% and 3.28%, respectively. Compared with the original performance, the initial filtration efficiency of DPF is improved by 16.42%. The optimized DPF pressure drop decreased by 15% and 36.33% at the beginning and end of the filtration period, respectively.

- **Keywords:** Diesel particulate filter; Multi-objective optimization; Sensitivity analysis; Response surface methodology; Analysis of variance

Yuh Nien Chow, Keng Yuen Foo. *Integrated assessment of phytotoxicity, stress responses, and bioaccumulative mechanisms of the arsenic-contaminated agricultural runoff using a soilless cultivation system*. Pages 266-280.

The present study has been oriented to the integrated assessment of physical, chemical, and physicochemical characteristics of the agricultural runoff (AR). The physical growth vigor, physiological and morphological changes, oxidative stress biomarkers, enzymatic and non-enzymatic antioxidative responses, elemental profiles, and bioaccumulative pathway of okra plant in relation to the changing concentrations of AR-induced irrigation were evaluated using a soilless cultivation system. Lindane, endosulfan, heptachlor epoxide, methoxychlor, hexachlorobenzene, chlordane, aldrin, heptachlor, dichlorodiphenyl-trichloroethane, and dieldrin were predominantly detected within the concentration range of 0.0025–0.069 μg/L, while arsenic, boron, copper, iron, manganese, and zinc were found at 0.63–25.50 μg/L. Concentration-dependent alterations of macroscopic symptoms, chlorophylls, morphological structures, reactive oxygen species, lipid peroxidation, protein oxidation, antioxidant enzymes, total phenolic content, and radical scavenging potential were recorded in the AR-irrigated groups. The accumulation of heavy metals were found in a descending order of: root>shoot>leaf>fruit. Specifically, arsenic was identified as the critical polluting species, as evidenced by the drastic interference in the uptake and metabolism of phosphate, calcium, potassium, and magnesium. The tolerable threshold concentration of 60% AR could be applied as a renewable source of irrigation water, verified by the negligible phytotoxic implications in the plant model.

- **Keywords:** Agricultural runoff; Arsenic; Bioaccumulation; Phytotoxicity; Soilless cultivation; Wastewater irrigation

Zeya Shen, Jianlei Lang, Mengzhen Li, Shushuai Mao, Feng Hu, Boyuan Xuan. *Impact of inlet boundary number and locations on gas diffusion and flow in a typical chemical industrial park near uneven terrain*. Pages 281-293.

Accurate simulation of pollution diffusion under uneven terrain with complicated obstacles is a difficult but important scientific and technological issue. The inlet-boundary was important and single boundary meteorological factors (e.g., wind direction and speed) input were generally employed for the Computational Fluid Dynamics (CFD) simulation. However, for uneven terrain with complicated obstacles, the boundary meteorological condition may be quite different, single boundary input may bring large simulation uncertainty. Consequently, the impact of different inlet boundary number and locations on CFD simulation was investigated based on a scarce tracer-gas field experiment carried out in a chemical industrial park located in a mountainous area. The experimental results implied gas diffusion was influenced by a combination of meteorological conditions from multi-inlet boundaries. The simulation results confirmed that and indicated commonly-used single-inlet boundary input can bring great inaccuracies. The case of inlet boundaries closed to emission sources and intersected the crosswind plane agreed best with measurements. It was also found that the inlet boundary number and locations significantly influence velocity and turbulence. Finally, a guideline for determining the inlet boundaries was proposed. This study can enhance the understanding on CFD simulation, and is beneficial for the selection of inlet meteorological sites to precise prediction.

- **Keywords:** Complex environment; Inlet boundary conditions; Gas diffusion and flow; Field experiment; Small scale

Xinxin Guo, Han Zhang, Xuhai Pan, Lijing Zhang, Min Hua, Chendong Zhang, Juan Zhou, Chenlu Yan, Juncheng Jiang. *Experimental and numerical simulation research on fire suppression efficiency of dry powder mediums containing molybdenum flame retardant additive*. Pages 294-308.

In order to cope with the frequent fire accidents in modern society, it is crucial to develop efficient fire extinguishing agents to stamp out fires in its early stage. In this work, a new composite ultrafine dry powder extinguishing agent containing ammonium molybdate ((NH4)2MoO4) is prepared, and its fire extinguishing efficiency is studied. The cup burner experimental results show that with the increase of the mass fraction of (NH4)2MoO4, the flame temperature drop and flame height variation rate show a trend of increasing and then decreasing, while the MEC and extinguishing time present a trend of a decrease and then an increase. It is indicated that the composite dry powder has the best fire extinguishing efficiency when the mass fraction of (NH4)2MoO4 is 7%. Besides, in terms of the pyrolysis results of TGA and DSC, it is found that the degree of thermal decomposition is significantly promoted under the condition of 7% addition. Based on the gas-solid two-phase flow theory and multiphase flow model, a simplified simulation model of the cup burner is established by the ANSYS-FLUENT software to analyze the variation of temperature and particle motion trajectory. The simulation results demonstrate that the ultra-fine dry powder mediums have a good dispersibility after entering the cup burner. This can achieve a full submerged state at a faster speed, and the flame temperature of the entire fire suppression stage is consistent with the experimental results. This article mainly develops the application of fire extinguishing media in the field of fire protection from the perspective of process safety.

- **Keywords:** Composite ultrafine powder; Flame retardant additives; Inhibitory efficiency; Pyrolysis mechanism; FLUENT; Particle trajectory

Peng Yang, Rongrong Hou, Danping Li, Rongfang Yuan, Fei Wang, Zhongbing Chen, Beihai Zhou, Huilun Chen. *Nitrogen removal from rural domestic wastewater by subsurface wastewater infiltration system: A review*. Pages 309-322.

Subsurface wastewater infiltration system (SWIS) has been widely used in rural decentralized sewage treatment due to its low cost, low energy consumption, high efficiency, and other advantages. Numerous researches have reported optimizing the SWIS nitrogen removal process, while the relevant mechanisms and optimization methods have not been well summarized. As such, this review aims to fill the above gaps as follows. Firstly, the SWIS nitrogen removal efficiency and mechanism are outlined, and the role of microorganisms is described in detail. Moreover, the issue of N2O emission in nitrogen removal was introduced. Secondly, the usage of different types of fillers in substrate improvement was summarized, highlighting the unique advantages of plants used in SWIS. A clear adjustment range and control method is proposed for system operating parameters such as hydraulic loading rate (HLR), organic loading rate (OLR), carbon-nitrogen ratio (CNR), temperature and dissolved oxygen (DO). Finally, the role of bioaugmentation in nitrogen removal was summarized. The part of conclusion and prospects evaluates the development and application of SWIS in rural areas.

- **Keywords:** SWIS; Rural domestic wastewater; Nitrogen removal; Microbial community; Influencing factors

Jude A. Okolie, Emmanuel I. Epelle, Meshach E. Tabat, Uzezi Orivri, Andrew Nosakhare Amenaghawon, Patrick U. Okoye, Burcu Gunes. *Waste biomass valorization for the production of biofuels and value-added products: A comprehensive review of thermochemical, biological and integrated processes*. Pages 323-344.

Waste biomass can be converted to green fuels and value-added products via thermochemical and biological conversion processes. The thermochemical processes endure limitations such as high processing costs due to high-temperature requirements. In contrast, the challenges of biological processes include low product yield and long processing time. Integrating different technologies, especially thermochemical and biological conversion processes, helps to enhance resource utilization and promote a circular economy. The combination of different technologies would help alleviate their limitations. In this respect, the integration of biological processes (e.g., syngas fermentation and anaerobic digestion) and thermochemical processes (e.g., pyrolysis, gasification, hydrothermal carbonization etc.) was the focus of this review. Integrated conversion processes often reduce the environmental impact compared to a standalone process. Hybrid pyrolysis-anaerobic digestion processes are promising from economics and ecological perspectives. However, more studies are required to understand how to effectively recycle and utilize the residue from pyrolysis and other thermochemical processes. Hydrothermal liquefaction (HTL) and pyrolysis are promising bio-oil production. However, HTL-derived oils are characterized by higher heating values and lower oxygen contents. The maturity level of most biological processes for waste biomass valorization is in the range of technology readiness level (TRL) 4–5. In contrast, thermochemical processes are expected to reach a TRL of 9 in the next two decades through detailed research and development. Moreover, the TRL of integrated processes described in the present study should also be assessed to evaluate their maturity and commercialization potential. The study will help researchers and policymakers to identify the knowledge gaps in integrating thermochemical and biological conversion processes. **Motivation and novelty statement:** The present review is the first of its endeavor to

present the advances, progress, and prospects of combining thermochemical and biological conversion processes for biofuels and value-added chemicals production. Most of the studies available in the literature focus on the advances in thermochemical or biological processes as a standalone conversion pathway despite many possible integration scenarios available. Therein lies the motivation for the present study. The current review is helpful for new researchers and policymakers to acquire the fundamental knowledge and possible pathways to unlock full biomass conversion pathways. Therefore, the authors made a significant effort to explain each conversion pathway in the first few sections before outlining their advantages and limitation. The final section was entirely on the different possible integration scenarios followed by process integration challenges. This study aims to open up the possibility of future research and help researchers identify the knowledge gaps in integrating thermochemical and biological conversion processes.

- **Keywords:** Circular economy; Biomass; Gasification; Biorefinery; Pyrolysis; Hydrothermal liquefaction; Anaerobic digestion; Syngas fermentation

Cheng-Chen Wang, Meng-Ying Li, Chang-An Yan, Wen Tian, Zhi-Hua Deng, Zhen-Xing Wang, Wu-Mei Xu, Yun-Fei Tuo, Ping Xiang. *Refining health risk assessment of heavy metals in vegetables from high geochemical background areas: Role of bioaccessibility and cytotoxicity*. Pages 345-353.

A systematic study of heavy metal levels, bioaccessibilities, and gastrointestinal cytotoxicity in two popular consumed vegetables mint (Mentha spicata Linn.) and pea sprouts (Pisum sativum Linn.) from three major producing cities in Yunnan, Southwest China were conducted for evaluating potential health risk to local inhabitants. The mean concentrations of As, Cd, Cr, and Pb were 0.34, 0.06, 1.04, and 0.79 mg/kg, respectively, with Cr and Pb exceeding 1.86–2.63 folds greater than the limit of Chinese National Standards and WHO/FAO. Their average gastric and intestinal bioaccessibilities varied within 12.1–59.4% and 9–53.3%, 0–93.3% and 0–82%, 41.8–71.1% and 19.1–62.9%, 16.1–93.6% and 9.5–81.7%, respectively. Cd in mint was the highest (86.8% and 39%, in the gastric phase and intestinal phase), while Pb had the highest bioaccessibility of 69.9% and 48.7% in pea sprouts. The bioaccessible target hazard quotient (BTHQ) of As, Cr, and Pb from vegetables reflected no potential health risks. However, toxicity assays showed intestinal digesta induced significant cytotoxicity in human intestinal Caco-2 cells, indicating the existing models based on total or bioaccessible heavy metals may be not accurate enough to assess their human health risk, especially for adverse effects evaluation. Taken together, the human risk assessment should be modified by taking their gastrointestinal cytotoxicity into account.

- **Keywords:** Vegetables; Heavy metals; Bioaccessibility; Health risks assessment; Caco-2 cells; Cytotoxicity

Quanwei Lv, Li'ao Wang, Jiaojiao Jiang, Shuda Ma, Lingyue Liu, Zili Zhou, Li Liu, Xiang Wang, Jisong Bai. *Catalytic pyrolysis of oil-based drill cuttings over metal oxides: The product properties and environmental risk assessment of heavy metals in char*. Pages 354-361.

Oil-based drill cuttings (OBDC), a hazardous organic waste generated from the exploration and extraction of shale gas fields, have received widespread attention for their safe disposal and utilization. In this study, OBDC pyrolysis experiments were conducted on a fixed-bed reactor. The effects of temperature (450 °C, 500 °C, 550 °C, and 600 °C) and catalysts (MgO, Fe2O3, and CaO) on product distribution, oil quality, and potential ecological risk assessment of heavy metals were investigated. Results revealed that the oil yield reached the maximum (14.94%) at 500 °C in uncatalyzed

cases. The addition of catalysts could increase the total yield of oil and gas. In particular, the oil yield increased by 13.32% with CaO catalysis, while the oil recovered by MgO and Fe2O3 was almost the same as without catalyst. In addition, the higher low heating value (LHV) of oil (41.46 MJ/kg) and gas (34.07 MJ/Nm3) were found with CaO catalysis, implying that CaO has better performance on recovery of oil and gas than MgO and Fe2O3. Moreover, the oil content of char was far below 0.3%, the potential ecological risk assessment of heavy metal in char showed slight risks to the environment, suggesting that char can be treated as general solid waste.

- **Keywords:** Oil-based drill cuttings; Pyrolysis; Oil; Heavy metal; Potential ecological risk

Lakhan Kumar, Mohita Chugh, Saroj Kumar, Krishna Kumar, Jaigopal Sharma, Navneeta Bharadvaja. *Remediation of petrorefinery wastewater contaminants: A review on physicochemical and bioremediation strategies*. Pages 362-375.

Wastewater generated at different stages of petrorefinery industry contains various toxic components including polyaromatic hydrocarbons, phenol, heavy metals, ammonia and other several hydrocarbons and non-hydrocarbons. These compounds remain in discharged wastewater as a complex which, when improperly treated and discharged into the environment, contaminates soils, aquifers, and groundwater. Prolonged exposure to such hazardous compounds even in minute amounts results in long term adverse effects on living beings. It gives rises to an array of pulmonary diseases like lung cancer and acute as well as chronic respiratory disorders. It may also lead to neurological toxicity, fatigue, headache and other psychiatric problems like anxiety and depression. The petrorefinery waste water treatment can be achieved by physical, chemical, and biological processes. Petrorefinery wastewater treatment can be done by physicochemical methods which are rapid but cause secondary pollution and are of cost-intensive in nature. Biological methods are comparatively slower, cheaper and environment friendly. In this review, we have studied different treatment technologies for petrorefinery wastewater with an emphasis on bioremediation strategies. Microbial consortia, genetically modified microbes and plants, a combination of plant and microbes, and specific purpose wetlands show promising results for petrorefinery wastewater treatment. An overview of petrorefinery wastewater composition and their harmful effect on environmental and public health and way forward has been presented.

- **Keywords:** Petrorefinery wastewater; Petroleum hydrocarbons; Environmental impact; Treatment strategies; Remediation; Bioremediation

Meng Qiao, Lujing Fu, Damia Barcelo. *Removal of polycyclic aromatic hydrocarbons by g-C3N4 nanosheets under visible light irradiation and effect of typical co-existence substances in river water*. Pages 376-381.

Polycyclic aromatic hydrocarbons (PAHs) ubiquitously exist in aqueous environment, posing considerable chronic and acute ecological risk to aquatic species. Non-metallic photocatalyst g-C3N4 is a promising photocatalyst that can be used in river remediation under visible light irradiation. The removal of a typical PAH phenanthrene (PHE) by g-C3N4 under visible light was detailed studied. The removal efficiency of PHE (initial concentration 5 mg/L) by g-C3N4-nano sheet (NS) (1 g/L) reached 100% within 10 min under visible light. Reactive oxygenated species, including •O2-, 1O2, and •OH, were generated in the g-C3N4-NS/visible light system. •O2- and 1O2 were determined as the main active species, whereas photoelectric-hole and •OH were also involved in the reaction. The effects of co-existed substances were investigated, including humic acid (HA), Cl-, and NO3-. HA decreased the removal rate of PHE, probably due to its reaction with photo-generated holes. Cl- with lower concentration (0.2 – 10.0 mmol/L) decreased

the removal rate of PHE, while with higher concentration (20 mmol/L) increased the removal rate of PHE, probably because of the interaction of Cl- with •OH. NO3- with the concentration of 10–100 μmol/L did not significantly affect the removal rate of PHE. This study will provide a possible in-situ route for the removal of typical PAHs in urban river environment.

- **Keywords:** Polycyclic aromatic hydrocarbons; Phenanthrene; G-C3N4 nanosheets; Humic acid; Cl-; NO3-

Leila Mohammadi Hadelu, Arshiya Noorpoor, Fateme Ahmadi Boyaghchi, Seyedali Mirjalili. *Exergoeconomic, carbon, and water footprint analyses and optimization of a new solar-driven multigeneration system based on supercritical CO2 cycle and solid oxide steam electrolyzer using various phase change materials*. Pages 393-421.

This study presents an innovative multigeneration for power, cooling load, distilled water, and hydrogen production from solar energy. The proposed system is comprised of a supercritical carbon dioxide (sCO2) ejector refrigeration cycle, a solar still desalination unit (SSDU), and a solid oxide steam electrolyzer (SOSE), integrated with parabolic dish collectors (PDCs) field. Exergoeconomic, carbon footprint (CF), and water footprint (WF) analyses are performed to assess the comprehensive performance of the system using seven inorganic and metal high-temperature PCMs, namely MgCl2, NaCl, LiF-MgF2, NaF-CaF2-MgF2, Zn-Cu-Mg, Cu-Si-Mg, and Cu-Si. It is found that Cu-Si delivers superior thermodynamic performance enhancement, and NaF-CaF2-MgF2 leads to the lowest economic, carbon, and water footprint performances among the desired PCMs. Moreover, multi-objective antlion optimization (MOALO) is conducted to ascertain and compare the maximum exergy efficiency and the minimum product cost, CO2 emission, and water consumption rates of Cu-Si and NaF-CaF2-MgF2. Under optimal conditions, Cu-Si gives an exergy efficiency of 31.27% with hydrogen, net power, cooling capacity, and distilled water production of 44.56 kg/h, 1508 kW, 74.03 kW, and 15.48 kg/h, respectively, and NaF-CaF2-MgF2 yields the lowest cost, CO2 emission, and water consumption rates of 73.55 $/h, 86.338 CO2e/h, and 180.73 kg H2O/h, respectively indicating 11.01%, 5.20% and 7.88% improvements with an 8.98% decrement in exergy efficiency compared with Cu-Si.

- **Keywords:** Exergoeconomic; Water and carbon footprint analyses; Supercritical CO2 cycle; Phase change material; Multi-objective antlion optimization

Dan Liu, Chunrong Wang, Zhipu Wang, Yixi Sun, Xianjie Liu, Shuang Xiao, Ling Li, Jiabin Zhou. *Magnetically separable NiFe2O4/sepiolite catalyst for enhanced ozonation treatment of quinoline and bio-treated coking wastewater in a catalytic ozonation system*. Pages 422-432.

In a quest to eliminate the bio-refractory organic pollutants in industrial wastewater, the NiFe2O4/SEP composites were synthesized via a sol-gel method and investigated by XRD, SEM, XPS, FTIR, VSM. The TOC removal increased from 16.82% to 69.35% in NiFe2O4/SEP+O3 system using quinoline as a target contaminant after 30 min, which is about 4.12 times as that in O3 system. The evolution of acetic acid, oxalic acid and formic acid in quinoline degradation was analyzed, saturated carboxylic acids were inertia to ozone molecules. However, 93.54% of oxalic acid was removed after 10 min, and 77.66% of acetic acid was degraded after 30 min in catalytic ozonation. The generation of small molecular organic acids could promote the Fe3+/Fe2+ redox cycle by complexing with Fe3+ on NiFe2O4/SEP, and then accelerated the formation of reactive oxygen species. In the presence of NiFe2O4/SEP, the high oxidation potential of •OH and •O2- contributed to an excellent TOC removal rate. Meanwhile, NiFe2O4/SEP was proved to be active for bio-treated coking wastewater in catalytic ozonation. The naturally

fluorescent constituents in bio-treated coking wastewater were almost entirely removed by NiFe2O4/SEP+O3 system in 60 min. These findings indicated the good potential of NiFe2O4/SEP for practical applications in industrial wastewater treatment.

- **Keywords:** Catalytic ozonation; Bio-treated coking wastewater; Mechanisms; Small molecular acids; Quinoline

Dongxu Ouyang, Jingwen Weng, Mingyi Chen, Jian Wang. *What a role does the safety vent play in the safety of 18650-size lithium-ion batteries?* Pages 433-441.

Herein, a series of experiments were performed to illustrate the impact of safety vents on the evolution of thermal runaway behaviors of 18650-size lithium-ion batteries. Meanwhile, the effect of safety vents on the thermal safety of batteries with different states of charge (SOC), i.e. 0%, 50% and 100% and cathode chemistries, i.e. lithium nickel manganese cobalt oxide (NMC), lithium cobalt oxide (LCO) and lithium iron phosphate (LFP) was explored. Compared with the battery with a safety vent, the thermal runaway behaviors of the battery in the absence of a safety vent are greatly worsened with ignition and thermal runaway occurring far earlier. As the battery SOC increases, it is demonstrated that the effect of the safety vent on battery thermal safety is reduced to some extent, with the difference in the times to thermal runaway between the batteries with and without a safety vent decreasing gradually. Besides that, it is found that the effect of the safety vent on the thermal runaway features of LFP-based batteries is relatively minor than in NMC-based batteries and LCO-based batteries. There is a linear-increasing relationship between the thermal runaway time difference and the mass loss difference for batteries with and without a safety vent.

- **Keywords:** Lithium-ion battery; Safety vent; Thermal runaway; Cathode chemistry

Sabrine Ghazouani, Faten Boujelbane, Dorra Jellouli Ennigrou, Bart Van der Bruggen, Nadia Mzoughi. *Removal of tramadol hydrochloride, an emerging pollutant, from aqueous solution using gamma irradiation combined by nanofiltration*. Pages 442-451.

Tramadol hydrochloride (TRAH) is an analgesic widely used in recent decades. This medicine is classified as an emerging contaminant, responsible for environmental damage and aquatic toxicity, that conventional wastewater treatment technologies are unable to successfully eliminate. This study focuses on TRAH degradation in aqueous solution by integrated methods of advanced oxidation and membrane filtration. Gamma irradiation was employed as advanced oxidation process (AOP) and the nanofiltration (NF) membrane was applied for the separation procedure. Indeed the degradation of TRAH solution by gamma irradiation was investigated by applying absorbed doses varying between 0.05 and 5 kGy. The experimental results indicate that at an initial concentration of 20 mg L−1, the maximum TRAH removal efficiency was 100% at 5 kGy while the removal efficiency of total organic carbon (TOC) was 78.7% at the same dose. NF enabled the rejection of TRAH and the efficiency did not exceed 90%. The integration of the two methods was then proposed and the results give 99.7%TRAH elimination and 81.5% TOC removal by a low absorbed dose of 0.4 kGy and applied pressure of 8 bar. The overall results show that the proposed coupled process in the first time is a suitable alternative for TRAH and TOC removal in an economic way with low energy consumption and sustainable as proven by the absence of chemical additives.

- **Keywords:** Tramadol hydrochloride; Emerging pollutant; Gamma irradiation; Nanofiltration; Degradation; Mineralization

Qingwei Xu, Kaili Xu. *Safety assessment of sand casting explosion accidents through on-site testing and numerical simulation of the temperature variation in sand molds to protect employee health*. Pages 452-463.

Sand casting explosion accidents will cause serious casualties, and measures should be adopted to prevent these consequences. The purpose of this study was to investigate the evolution mechanism of sand casting explosion accidents. The temperature variations in sand molds were investigated based on on-site testing and numerical simulation. The evolution characteristics of sand casting explosion accidents were analyzed by fault tree analysis, chaos theory and synthetic theory model. The results showed that the temperature at the monitoring point rose rapidly once the energy of molten steel was transferred to the sand mold and then dropped slowly. The closer the monitoring point is to the interface of the casting, the higher the temperature is at the monitoring point. The moisture content in the sand mold is a key factor for sand casting explosion accidents. Sand casting explosion accidents exhibit sensitivity and inherent randomness and are affected by employee, object, environmental and management factors. The organizational factors of sand casting explosion accidents are remote causes, and social factors are basic causes. The findings with respect to sand casting explosion accidents can be regarded as the foundation of accident prevention in practice.

- **Keywords:** Sand casting explosion accidents; On-site testing; Numerical simulation; Fault tree analysis; Chaos theory; Synthetic theory model

Huan Zhang, Bing Wang, Chunyang Gao, Tianju Zhu, Mingyang Xiong, Hongyang Ren. *Effective degradation of hydrolyzed polyacryamide (HPAM) in a simultaneous combination of acoustic cavitation and microbubbles ozonation: Process optimization and degradation mechanism*. Pages 465-476.

Managing environmental contamination with hydrolyzed polyacryamide (HPAM) is essential due to its persist long with slow biodegradability influence on the environment. In this study, the simultaneous combination of acoustic cavitation and microbubbles ozonation (US/O3) was applied to generate additional highly reactive hydroxyl radicals (·OH) and thus to enhance the degradation of HPAM. Compared with the two separated degradation process methods, the coupled method exerts a synergistic effect on the decomposition of HPAM, with an enhancement factor of 1.50. Effects of aeration pattern, ultrasound irradiation, operating temperature, initial HPAM concentration, and valance state of cations on the removal of HPAM were investigated intensively. An increase in valance state of cations contributes to HPAM removal. The maximum HPAM degradation, chemical oxygen demand (CODcr) removal and viscosity reduction of the HPAM wastewater were 97.35%, 89.01% and 93.25%, respectively. The degradation of HPAM conformed to the first-order reaction kinetic model. Removal of HPAM followed hydroxyl radical mechanism. The degradation mechanism of HPAM was also discussed with the change of FTIR and UV–Visible spectra of HPAM in investigated processes. The main reaction intermediates, such as heptanoic anhydride, oleamide, myristamide, acetic acid, acetamide, and propanamide, are identified and a possible degradation pathway is proposed during the US/O3 process. The process was proved to be a suitable technique for dealing with HPAM-containing wastewater.

- **Keywords:** Hydrolyzed polyacryamide; Acoustic cavitation; Ozonation; Cations; Hydroxyl radicals

Chukwuma Nnaji, Ziyu Jin, Ali Karakhan. *Safety and health management response to COVID-19 in the construction industry: A perspective of fieldworkers*. Pages 477-488.

The COVID-19 outbreak has significantly impacted the construction industry. The pandemic can exacerbate an already dire safety and health situation in the industry and negatively impact construction employees and employers. The present study investigates the safety and health measures implemented by construction firms in the United States (US), their effectiveness and usefulness, and workers' satisfaction with these COVID-19 measures. A questionnaire survey was developed and distributed to construction fieldworkers in the US to collect their perspectives on the implemented COVID-19 measures in the construction industry. A total of 187 valid responses were received and analyzed to achieve the aim of the study. Results revealed that strategies implemented to increase social distance and minimize group gathering to 10 persons in certain workstations were perceived to be substantially more effective than job-site screening strategies. Furthermore, smaller contractors implemented fewer safety measures and perceived them to be significantly less effective than those used by medium- and large-sized contractors. Fieldworkers were favorably disposed toward using technologies, such as video-conferencing apps and wearable sensing devices, to slow the spread of COVID-19 on construction job sites. The present study contributes to the body of knowledge by identifying safety and health measures to mitigate the spread of COVID-19 in construction. Practically, the study findings provide valuable insights to inform the successful implementation of safety strategies in the construction industry during a pandemic. The results are crucial for industry practitioners responsible for developing and revising pre- and post-pandemic safety and health plans.

- **Keywords:** COVID-19; Pandemic; Coronavirus; Construction management; Safety and health; Strategies; Technologies

Sahar T. Mohammed, Saba A. Gheni, Dhia Y. Aqar, Khaleel I. Hamad, Safaa M.R. Ahmed, Marwan A. Mahmood, Ghassan H. Abdullah, Mustafa K. Ali. *Evaluation and optimal design of a high stability hydrothermal deoxygenation process for production of green diesel fuel via deoxygenation of waste cooking oil*. Pages 489-499.

The environmental impacts of waste cooking oil (WCO) can be profoundly serious when it is not handled properly. Instead of discarding leftover cooking oil as waste, recent technological advancements have made it possible to use WCO as a sustainable feedstock for biofuels production, while also addressing the disposal issue. This work developed an efficient and high stability hydrothermal WCO transformation process into green diesel fuel. In the present work, a homemade environmentally benign activated carbon was prepared from a bio-sourced precursor and impregnated with a Pd precursor. A set of experiments were conducted at 300 °C–350 °C, 40 and 50 bar, and times up to 240 min to evaluate the performance of Pd/AC catalysts against deoxygenation (DO) and deactivation reactions. The results showed a substantial enhancement of the activity and stability of the coated Pd/AC catalyst versus the uncoated one. Also, the green diesel fuel possesses an outstanding higher heating value of 46 kJ/mol. Based on experiments, the best kinetic model for the DO process was developed. The optimum kinetic parameters were obtained by the optimization approach. For a wide variety of operating conditions, the projected product conversion demonstrated satisfactory agreement with the experimental results, with absolute average errors of less than 8%.

- **Keywords:** Green diesel fuel; Hydrothermal deoxygenation; Waste cooking oil; Optimal design; Stability

Fatemeh Amir Aslanzadeh Mamaghani, Amin Salem, Shiva Salem. *Pilot plant study for management of toxic solid waste collected in landfill of spent lubricant oil refinery by conversion into zeolite packed bed via continuous extrusion and fusion techniques*. Pages 500-510.

The pilot plant extrusion was successfully utilized to manage a clay based solid waste deposited in the landfill of spent oil refinery through the conversion into the rod-like zeolite with LTA (Linde Type A) structure. The research was designed in combination with fusion, and hydrothermal processes to produce a packed bed with appropriate cation exchange capacity (CEC). However, the conversion of waste into the proper zeolite structure was the challenge of study due to lack of aluminum. To address this issue, boehmite, and sodium hydroxide were added to solid waste for compensation of aluminum lack before extrusion. The extrudates were further consolidated by fusion at 800 °C, and then were converted into zeolite LTA by control of aging, and reaction periods in the hydrothermal step. The crystallinity, microstructure, and textural characteristics of waste, and fabricated rods were studied to examine the capability of process. The results revealed that the rod fabricated through the short aging period, 3 h, and longer reaction time, 9 h, represents the minimal CEC due to the recrystallization of hydroxysodalite. Although the textural characteristics of zeolites were found to be slightly affected by extrusion, the aging, and reaction periods of 9, and 6 h are beneficial to produce a packed bed with proper CEC, 214 mg g−1, demonstrating the potential of innovated technique.

- **Keywords:** Clay based waste; Spent lubricant oil; Extrusion; Fusion; Zeolite LTA; Cation exchange

Fikret Polat, Murat Kadir Yeşilyurt, Ümit Ağbulut, Mustafa Karagöz, Suat Sarıdemir. *Experimental assessment of the influences of liquid-solid-gas fuel blends on DI-CI engine behaviors*. Pages 511-524.

This study aims to deeply investigate the effects of the boron nanoparticles reinforced diesel fuel along with various biogas (BG) flow rates (0.5, 1, and 2 L/min) on the engine performance and emission characteristics of a diesel engine. The tests were carried out using a single-cylinder, four-stroke, direct injection, compression-ignition engine at a constant engine speed of 1500 rpm and under the varying engine loads from 2.5 to 10 Nm with gaps of 2.5 Nm. In the results, it is seen that EGT started to decrease in both the addition of boron nanoparticles and the addition of biogas compared to that of conventional diesel fuel (DF). EGT reduced by 8.6% for DF+Boron test fuel, 14.4% for DF+Boron+ 0.5 BG, 21% for DF+Boron+ 1 BG, and 23.4% for DF+Boron+ 2 BG. Compared to diesel fuel, CO, NOx, and HC emissions decreased with the addition of nanoparticles at all loads. However, as the amount of biogas increased, CO and HC emissions increased, but NOx emissions decreased. CO emission dropped by 22.2% for DF+Boron test fuel, however, increased to be 5.6%, 16.7%, and 36.1% for DF+Boron+ 0.5 BG, DF+Boron+ 1 BG, and DF+Boron+ 2 BG respectively. NOx emission reduced by 4.9%, 8.6%, 10.7%, and 14.8% for DF+Boron, DF+Boron+ 0.5 BG, DF+Boron+ 1 BG, and DF+Boron+ 2 BG respectively. In comparison to that of conventional DF, the brake specific fuel consumption (BSFC) value decreased by 8.42% for DF+Boron test fuel due to high energy content of nanoparticles, but it increased by 10.94% for DF+Boron+ 0.5 BG, 28.01% for DF+Boron+ 1 BG, and 60.2% for DF+Boron+ 2 BG. In addition, brake thermal efficiency BTE value increased by 8.04% for boron-added test fuel, but it declined by 9.41% for DF+Boron+ 0.5 BG, 19.38% for DF+Boron+ 1 BG, and 32.2% for DF+Boron+ 2 BG as compared to that of DF. In the conclusion, it is noticed that the engine characteristics have worsened by the introduction of biogas into the cylinder, but these worsened characteristics can be improved with the presence of boron nitride nanoparticles.

- **Keywords:** Boron nanoparticles; Biogas; Nanofuel; Engine performance; Exhaust emissions

Minju Cha, Chanhee Boo, Chanhyuk Park. *Simultaneous retention of organic and inorganic contaminants by a ceramic nanofiltration*

***membrane for the treatment of semiconductor wastewater*. Pages 525-533.**

The semiconductor manufacturing industry produces large amounts of ammonia-contaminated wastewaters which require costly and energy-intensive treatments. This study demonstrates the application of a commercially available ceramic nanofiltration (NF) membrane for the control of organic and inorganic contaminants as well as ammonium retention in the treatment of semiconductor wastewater. Analysis of the hydrodynamic pore transport model based on the direct measurement of membrane thickness in the active layer indicated that the ceramic NF membrane has an average pore radius of ≈0.65 nm. Zeta potential measurements of the ceramic NF membrane showed that the membrane surface was negatively charged at neutral pH. The ammonium retention capacity of the ceramic NF membrane was evaluated using a single symmetric ammonium salt solution (1.8 mM NH4HCO3; i.e., the average ammonium concentration in semiconductor wastewater) and combined salt solutions (mixtures of 1.8 mM NH4HCO3 and either 2.0 mM of Na2SO4, CaSO4, or CaCl2). The combined NH4HCO3 and Na2SO4 solution rendered a remarkably high ammonium retention rate of 88.7%, which was attributed to higher valency co-ions (SO42-) in this solution with the same negative surface charge of the ceramic NF membrane. In contrast, the calcium ions (Ca2+) in different combined salt solutions containing CaSO4 and CaCl2 interfered with ammonium retention. We further employed the ceramic NF membrane to treat semiconductor wastewater samples taken from a full-scale semiconductor wastewater treatment plant and demonstrated that this proposed treatment method could effectively retain organic and inorganic contaminants with a low fouling propensity. Our results highlight the promising potential of ceramic NF membranes for the treatment of industrial wastewaters with diverse organic and inorganic contaminants.

- **Keywords:** Ammonium; Ceramic nanofiltration membrane; Organic and inorganic contaminants; Retention mechanism; Semiconductor wastewater

Huilin Li, Yi Zheng, Qiu Yu, Binquan Jiao, Dongwei Li. *Optimization for enhanced electrokinetic treatment of air pollution control residues using response surface methodology focusing on heavy metals leaching risk and extractability*. Pages 534-546.

Waste like air pollution control (APC) residues from incineration are potentially valuable resources. This paper reports the application of enhanced electrokinetic (EK) treatment processing to APC residues using an approaching anode coupled with a permeable reactive barrier (PRB). The changes of heavy metals (HMs) leaching risk and the effect of EK on metals extractability were explored for the possibilities of treated APC residues and metals recovery. The impact of various factors on HMs leaching was evaluated through response surface experiments. The adsorption ability of PRB and H+ provided by approaching anode could alleviate HMs accumulation during treatment caused by high pH and buffer capacity. Compared with conventional EK treatment, the HMs extraction and leaching reduction improved significantly, with more than 30% energy saved after enhanced EK treatment. The best HMs leaching reduction was obtained after 16 days treatment at 1.97 V/cm of voltage gradient with 14.64 g modified activated carbon used as PRB while the anode was moved after 6.35 days. The results showed fraction conversions could increase the extractability of HMs with the electric field application, and the environmental risk of remaining HMs was reduced through the effective removal of HMs with potential risk after enhanced EK treatment.

- **Keywords:** Electrokinetic treatment; Air pollution control waste; Response surface methodology; Heavy metals; Leaching risk

Binbin Huang, Min Gan, Zhiyun Ji, Xiaohui Fan, Dan Zhang, Xuling Chen, Zengqing Sun, Xiaoxian Huang, Yong Fan. *Recent progress on the thermal treatment and resource utilization technologies of municipal waste incineration fly ash: A review*. Pages 547-565.

Incineration is becoming a promising and effective approach to dispose the increasing municipal solid waste, while the fly ash produced is another urgent problem needed to be addressed. Municipal solid waste incineration fly ash (MSWI-FA) contains heavy metals and organic pollutants, which exert huge threat to human health and environmental safety. This paper analyzed the current situation of MSWI-FA, summarized the technologies of hazard-free treatment and resourceful utilization, expounded its future development trend. The latest thermal detoxification technologies of MSWI-FA were reviewed, including melting/vitrification, hydrothermal treatment and thermal plasma technology. The organic pollutants can be efficiently decomposed during the thermal treatment process, and the heavy metals can be stabilized, which was currently the most effective hazard-free treatment technology. The resource utilization technologies of MSWI-FA related to thermal treatment, including the application of MSWI-FA in the production of asphalt, cement, and glass ceramics, were reviewed. The life cycle assessment of various MSWI-FA treatment technologies were summarized and compared. The main principle was to make full use of the physicochemical characteristics of MSWI-FA, with its purpose to realize value-added utilization, and to decompose and stabilize the hazardous components during high-temperature process. The mechanism and technical characteristics of treating MSWI-FA through thermal detoxification and resource utilization were deeply summarized, and the future research work that needs to be further strengthened was proposed, thereby promoting the safe and effective treatment of MSWI-FA and realizing the green and sustainable development of the city.

- **Keywords:** MSWI-FA; Thermal treatment; Hazard-free treatment; Resource utilization; Green and sustainable development

Hideo Maruyama, Hideshi Seki. *Recovery of milk whey proteins by foam separation*. Pages 566-574.

Milk whey proteins recovery was conducted with foam separation. Experiments were conducted by batch mode in pH 4–8. The separation rate was evaluated by the rate constant of the first-order kinetic equation. Both recovery efficiency and separation rate were highest at pH 7. Overall equilibrium adsorption constant, K, and saturated adsorption density, Xs, were determined from a proposed estimating method using data obtained in batch mode. At pH 7, K and Xs were determined using the data obtained in continuous mode. K and Xs determined by both operation modes were agreed well. Adsorption parameters of the major proteins in milk whey (bovine serum albumin (BSA), α-lactalbumin (LA), and β-lactoglobulin (LG)) were estimated by the proposed estimating method in pH 4–7. Xs is largest at pH 5 and the K of LG over pH 5 was larger, which suggested that LG was the most hydrophobic species among them.

- **Keywords:** Foam separation; Milk whey protein; Adsorption; Water treatment; Bio-resource recovery

Qiusheng Song, Peng Jiang. *A multi-scale convolutional neural network based fault diagnosis model for complex chemical processes*. Pages 575-584.

The chemical production process is a special dynamic and complex system. It has the characteristics of instability and danger, thus making safety management in the production process very difficult. To support the long-term and stable operation of the chemical process, timely and accurate fault diagnosis is very necessary. Aiming at the

high-dimensional nonlinearity of chemical process data, this paper proposes a fault diagnosis method in chemical process that is based on multi-scale convolutional neural network (MsCNN) combined with matrix diagram. This model uses software to convert the pre-processed time series signal data of the chemical process into sets of matrix diagrams, and then uses the MsCNN model to accurately diagnose various types of faults in the chemical production process. Taking Tennessee Eastman (TE) process fault data set as an example, verification shows good simulation results in detection accuracy and loss. This method can create high-precision judgments on fault types, which is beneficial to timely elimination of faults and avoidance of safety accidents. The results show that the new model proposed in this paper has good potential in the field of fault diagnosis in chemical processes, and is also reliable, practical and scientific.

- **Keywords:** Multi-scale convolutional neural network (MsCNN); Chemical process; Fault diagnosis; Matrix diagram; Tennessee Eastman process

Hamidreza Seiti, Ahmad Makui, Ashkan Hafezalkotob, Mehran Khalaj, Ibrahim A. Hameed. *Graph: A new risk-based causal reasoning and its application to COVID-19 risk analysis*. Pages 585-604.

Various unexpected, low-probability events can have short or long-term effects on organizations and the global economy. Hence there is a need for appropriate risk management practices within organizations to increase their readiness and resiliency, especially if an event may lead to a series of irreversible consequences. One of the main aspects of risk management is to analyze the levels of change and risk in critical variables which the organization's survival depends on. In these cases, an awareness of risks provides a practical plan for organizational managers to reduce/avoid them. Various risk analysis methods aim at analyzing the interactions of multiple risk factors within a specific problem. This paper develops a new method of variability and risk analysis, termed R.Graph, to examine the effects of a chain of possible risk factors on multiple variables. Additionally, different configurations of risk analysis are modeled, including acceptable risk, analysis of maximum and minimum risks, factor importance, and sensitivity analysis. This new method's effectiveness is evaluated via a practical analysis of the economic consequences of new Coronavirus in the electricity industry.

- **Keywords:** R.Graph; Risk analysis; Causal chain; COVID-19

Nevim Genç, Elif Durna Pişkin, Şeyda Aydın. *Optimization of ZVAl based oxidation and reduction process conditions: Selection of the most suitable process by multiple-criteria decision-making approach*. Pages 605-615.

The use of zero valent aluminum (ZVAl) has attracted attention as an effective agent in the oxidation and reduction of pollutants due to its electron donor nature. In this study, the removal of the target pollutant Sunfix red S3B (SR-S3B) azo dye with ZVAl based processes was investigated. For maximum dye removal efficiency, the operating conditions of the processes are optimized with Box Behnken Design. With the optimum conditions of the (PS+ZVAl) oxidation process (PS dose of 12.5 g anion/L, duration of 134 min, pH of 2, ZVAl dose of 3.5 g/L) 94.95% dye removal, and with the optimum conditions of the (H2O2+ZVAl) oxidation process (H2O2 dose of 0.20 M, duration of 180 min, pH of 2, ZVAl dose of 1.44 g/L) 55% dye removal efficiency was obtained. In the (O2 status+ZVAl) reduction process, 77.27% dye removal efficiency was obtained under optimum conditions (anaerobic conditions, duration of 14.8 min, pH of 2, ZVAl dose of 1.43 g/L). With the Pareto analysis of (PS+ZVAl), (O2 status+ZVAl) and (H2O2+ZVAl) processes, the parameters with the highest effect were determined as (ZVAl dose)2 (37.42%), O2 status (29.56%), and (H2O2xpH) (28.38%) respectively. The optimized processes were evaluated by the PROMETHEE method, taking into account

the criteria of dye removal efficiency, operating cost and possible residues of oxidizing/reducing agents. The preference ranking of the processes was determined as (O2 status+ZVAl)> (PS+ZVAl)> (H2O2+ZVAl).

- **Keywords:** Zero valent aluminum; Oxidation; Reduction; Process optimization; PROMETHEE

Lipin Li, Huan Chen, Yanqun Huang, Guochao Xu, Pengli Zhang. *A new small leakage detection method based on capacitance array sensor for underground oil tank*. Pages 616-624.

The early detection and discovery of small leakages from underground storage tanks (USTs) is an effective means for preventing the spread of contamination to deep soil and groundwater, which is of great significance to the process safety and risk management of oil tanks. In the previous studies, the soil sample collecting by these boreholes near the oil tank, the detection results have a certain degree of randomness and non-timeliness due to the sampling affected by the distribution of the boreholes, which would result in failure to catch small leakages of UST in time. According to capacitance sensor having a sensible capacity for relative permittivity of the soil, we propose a new small leakage detection method that employs the full-coverage three-dimensional capacitance array sensor with optimized parameters and higher sensitivity and our established measurement function of oil leakage to realize early detection of small leakage. Such a method can effectively solve the problems of incomplete sampling and easy to miss small leaks in borehole sampling detection. In addition, the experimental results show that the absolute error is less than 0.110% when selecting the small oil leakage in the range of 0.068~3.261%. Therefore, our method has higher measurement accuracy and could offer an efficient way for early discovery and quantitative estimation of small oil leakages from UST, which would provide a reliable basis for process safety and risk prediction.

- **Keywords:** Small oil leakage; Capacitance array sensor; Underground storage tank; Early detection

Lei Zhao, Junjie Liu, Yihui Yin, Jingjing Pei, Wu Xiao, Haiqiao Zhang, Shen Wei. *Field investigation of pollutant characteristics and targeted ventilation control strategies in high-ceiling aircraft spraying workshop*. Pages 627-639.

To achieve efficient ventilation and purification in the high-ceiling painting workshop is faced with the contradiction between effect and energy consumption. Understanding the characteristics of gaseous pollutants is of paramount importance for ventilation and purification system design. The composition and concentration of volatile organic compounds (VOCs) emitted from aircraft painting workshop were sampled by Tenax-TA tubes and analyzed with gas chromatography-mass spectrometry (GC-MS). Approximately 50 types of VOCs (detection rate>50%) were detected in the aircraft spraying workshop, with percentages of 36.3% for esters, 31.9% for aldehyde ketones, 28.5% for biphenylenes, 1.9% for alcohols and 1.4% for alkanes. The TVOC concentrations in the workshop were 48.6 mg/m3 and 132.4 mg/m3, during the varnish painting and the finish painting processes, respectively, and these are several times higher than those observed in other industries (automobile painting and wooden furniture painting). The field test data of spraying workshops from 197 spraying factories in five industry sectors were collected from field measurement and existing literature. Some VOCs components are the general pollutants in the painting workshops, such as Acetic acid, butyl ester, Toluene, and 2-Butanone. A novel ventilation model using multiple target purification units is proposed to eliminate the pollutants in an aircraft spraying workshop. Compared with the original trench exhaust system, the air volume of the

proposed targeted ventilation system is reduced by 75%, and the energy consumption is reduced by 45,000 kW·h per aircraft.

- **Keywords:** Aircraft spraying workshop; VOCs; Targeted ventilation; Field test; Pollution control

Kendric Aaron Tee, Mohammad A.H. Badsha, Musharib Khan, Ka Chun James Wong, Irene M.C. Lo. *Lanthanum carbonate nanoparticles confined within anion exchange resin for phosphate removal from river water: Batch and fixed-bed column study*. Pages 640-651.

The use of lanthanum for phosphate removal has gained increasing attention due to its relative abundance, non-toxicity, and strong affinity toward phosphate. In this regard, although lanthanum hydroxide exhibits promising phosphate removal ability, its practical application remains limited due to certain technical issues including its structural instability and leaching. To circumvent these issues, a lanthanum carbonate-based adsorbent was developed in this study. Lanthanum carbonate@anion exchange resin (LC@AER) and lanthanum hydroxide@anion exchange resin (LH@AER) beads were first prepared through in-situ precipitation using identical bead-to-precursor mass ratios. LC@AER beads were chosen for further study as they displayed better adsorption capacity and stability, and the bead-to-precursor mass ratio was further optimized to improve performance and stability. LC@AER (1:2) beads exhibited a maximum adsorption capacity of 77.43 mg-P/g and excellent selectivity toward phosphate in the presence of various co-existing anions. Experiments using river water indicated high phosphate removal efficiency, demonstrating potential for treating river water. Investigations revealed key differences in phosphate binding mechanisms for batch and column experiments. In batch setting, phosphate is primarily captured through ligand exchange and inner-sphere complexation. However, over prolonged column operation, surface precipitation and electrostatic attraction (between phosphate and quaternary ammonium) become increasingly important for binding phosphate, which may affect phosphate recovery efficiency and must be accounted for in process design. Overall, the findings indicate that lanthanum carbonate serves as a good alternative to lanthanum hydroxide and that LC@AER (1:2) beads are promising for phosphate removal.

- **Keywords:** Fixed-bed column; Lanthanum carbonate; Nanocomposite beads; Phosphate; Sorption

Geraldo Cardoso de Oliveira Neto, Henrricco Nieves Pujol Tucci, Moacir Godinho Filho, Wagner Cezar Lucato, Dirceu da Silva. *Moderating effect of OHS actions based on WHO recommendations to mitigate the effects of COVID-19 in multinational companies*. Pages 652-661.

The objective of this study was to evaluate the moderating effect of Occupational Health and Safety actions based on the World Health Organization (WHO) recommendations to mitigate the negative effect of COVID-19 on the operational, logistical, marketing (OLMP), and health and safety performance (OHSP) of workers in multinational industries. The development of surveys in companies was the method adopted, which had confirmatory evaluations through Structural Equations Modelling (SEM). As a result, it was confirmed that this is one of the few scientific studies that expectedly validates that the COVID-19 pandemic has severely impacted operational, logistical, market, and Occupational Health and Safety (OHS) performance. This is also one of the few research projects to assess the moderating effect of OHS practices based on WHO to mitigate the effects of COVID-19. According to our findings, those practices were able to reduce by at least 50% the effect of the COVID-19 crisis on operational, logistical, and marketing performance. However, they minimize by only 1.8% the negative effects of health and safety performance for the worker, generating absenteeism increasingly due to physical

and mental problems. This number could be higher if the social distance could be provided in public transportation and if employees were more aware of the risks of COVID-19 contamination during their social activities.

- **Keywords:** Occupational Health and Safety; COVID-19; Performance

Kai Zheng, Juncheng Jiang, Zhixiang Xing, YongMei Hao, Minggao Yu, Xufeng Yang, Yuwei Tao. *Application of large eddy simulation in methane-air explosion prediction using thickening flame approach*. Pages 662-673.

In this work, large eddy simulation (LES) is carried out to investigate the stoichiometric methane-air explosion through using thickening flame model. The power-law model is used to evaluate the efficiency factor and a reduced two-step combustion mechanism is considered for the methane-air combustion. The adaptive grid refinement is adopted and different thickening factors are simulated. The numerical model is validated by comparing the predicted results with experimental data. It is seen that the numerical model can reproduce the experiment data quantitatively and qualitatively. All the stages of tulip shaped flame are well repeated by LES in both 2D and 3D forms. For the flame propagating in smooth duct with tulip shaped flame formation, the effect of efficiency factor can be ignored due to its small value. The thickening factor should be estimated through using thermal thickness of premixed flame and it needs to ensure that the thickened flame can cover at least 5 grid cells. The ignition radius needs to be larger than the thickness of thickened flame to ensure the premixed flame to grow steady after the ignition.

- **Keywords:** Methane/air; Large Eddy simulation; Thickening flame; Explosion

Jiawei Sun, Haiyang Jia, Hengchang Bi, Miaoling Que, Lixiang Chen, Qiubo Zhang, Yuwei Xiong, Xiao Xie, Yunfei Sun. *Laser-assisted synthesis of graphene-based paper for both oil/water mixtures and emulsions separation*. Pages 674-684.

Nowadays, dealing with the complex oil/water contamination that contains both oil/water mixtures and emulsions with desirable performance remains a huge challenge. Complicated fabrication procedures, low flux, and efficiency are shortcomings of the known materials. Herein, a facile and effective laser-assisted strategy is proposed to prepare super-hydrophobic graphene/PDMS paper (L-G-P), which perfectly takes advantage of both naturally strong capillary of paper tissue and high-quality graphene. Specifically, graphene is obtained by reducing graphene oxide via laser irradiation, which avoids introducing chemical reducing agents that are either hazardous or hard to separate. Meanwhile, the super-intensive instantaneous energy would create abundant defects on graphene sheets, thus the specific surface area increased by 25%. As for oil/water mixtures, the efficient sorption/separation can realize over 99.99% deep clean, meanwhile showing excellent durability after repeated cycles. As for water-in-oil emulsions, the high separation flux of surfactant-stabilized emulsions could reach 4421 L m−2 h−1 with an efficiency up to 99.85%. Moreover, the mechanical property of the composite was 80.50% stronger than uncoated paper tissue. The proposed L-G-P with durable and efficient oil/water separation performance is a promising material for practical applications for treating oil-contaminated wastewater in harsh environments.

- **Keywords:** Laser-assisted; Graphene-based; Superhydrophobic; Oil/water mixtures separation; Emulsions separation

Jiangyuan Qu, Nana Qi, Kai Zhang. *CFD modeling for NOx absorption accompanying with SO2 in wet flue gas desulfurization scrubber based on gas-phase ozone oxidation*. Pages 685-697.

NOx removal performance accompanying with SO2 is investigated in a two-step process containing O3 pre-oxidation of NO and NOx post-absorption in the scrubber of wet flue gas desulfurization (WFGD) unit. Based on EulerianLagrangian framework, a comprehensive CFD model is established to describe the reactions of NO2 and N2O5 with S(IV) in droplets coupled with NOx transfer process and hydrodynamics in the scrubber. Taking the WFGD scrubber of 330 MW coal-fired power unit as case study, the results indicate NOx absorption efficiency in scrubber is increased by increasing O3/NO molar ratio from 1.0 to 2.2 and decreasing reaction temperature from 423 K to 363 K in O3 pre-oxidation process. The obtained highest removal efficiency is 85.79% for pH of 5.5 or 96.32% for pH of 9.0 in droplets. NO2 absorption is much slower than N2O5 and more sensitive to chemical compositions in droplets or hydrodynamics in scrubber. The overall mass transfer coefficient (KG) for NO2 is mainly determined by pH and S(IV) concentration in droplets, while the specific interfacial area (a) is largely influenced by gasdroplet hydrodynamics in scrubber. Finally, a correlation is proposed to predict the volumetric mass transfer coefficient (KGa) for NO2 absorption accompanying with SO2 in WFGD scrubber.

- **Keywords:** Nitrogen oxides; Ozone pre-oxidation; Wet flue gas desulfurization; Two-phase flow; Absorption; Eulerian-Lagrangian model

Hengfei Zou, Jingqi Yuan. *Online application oriented dynamic modeling for the flue gas desulfurization tower in coal-fired power plants*. Pages 698-707.

A dynamic model for the flue gas desulfurization tower in coal-fired power plants is proposed. The model is validated with the data from a 350 MW unit. The penetration theory is adopted in modeling. The movement and the size of the slurry droplets, the temperature and the flow rate of the flue gas, as well as the chemical reactions have been taken into account. Three parameters in the model are found to have a critical impact on the model accuracy, i.e., the droplets' initial velocity, the number of droplets leaving all nozzles in a single spray layer per unit time, and the liquid side mass transfer coefficient of sulfur dioxide. These parameters need to be identified periodically in real applications. The quantitative relationship between pH and liquid side mass transfer coefficient is given. The main hypotheses and parameters of the model were discussed in order to quantify their respective influence. The model may be used to simulate the desulfurization process across the entire load range. Specifically, it may be used to predict the desulfurization efficiency online, so that applied potentially for the operational optimization.

- **Keywords:** Coal-fired power plants; Wet flue gas desulfurization; Dynamic modeling and validation; Estimation of the desulfurization efficiency

Dandan Gong, Yong Zhang, Linsheng Wan, Tingsheng Qiu, Yunnen Chen, Sili Ren. *Efficient extraction of tungsten from scheelite with phosphate and fluoride*. Pages 708-715.

Considering the problems of high temperature and large reagent consumption in the current alkali decomposition processes, phosphate and fluoride were adopted to extract tungsten from scheelite. The results indicated that tungsten could be efficiently extracted with a decomposition rate of> 98.0% under moderate decomposition conditions, forming fluorapatite in the decomposition residue. The decomposition yield is influenced by the calcium fluoride dosage, decomposition temperature, liquid-to-solid ratio, and holding

time. Furthermore, the decomposition reaction followed the surface chemical reaction controlling step. Additionally, the phosphorus concentration in the decomposition solution was lower than 0.2 g/L. This work may provide an alternative for the efficient tungsten extraction from scheelite, especially fluorite bearing scheelite under relatively low reagent costs and temperature.

- **Keywords:** Scheelite; Decomposition; Phosphate; Fluoride; Fluorapatite

Sayeh Yasamani Masouleh, Mehrdad Mozaffarian, Bahram Dabir, Saeed Fallah Ramezani. *COD and ammonia removal from landfill leachate by UV/PMS/Fe2+ process: ANN/RSM modeling and optimization*. Pages 716-726.

Landfill leachate is a highly contaminated liquid generated in municipal solid waste landfills. The application of sulfate radical-based advanced oxidation processes (SR-AOP) in landfill leachate treatments is emerging due to their ability to degrade both organic refractory matters and ammonia nitrogen. In this paper, application of peroxymonosulfate (PMS), activated by Fe2+ and UV was used as an economical and environmentally friendly approach for treatment of landfill leachate. Chemical oxygen demand (COD) and ammonia removals were measured as the two primary responses of landfill leachate to UV/PMS/Fe2+ treatment system. The main parameters (pH, PMS/Fe2+ mass ratio, Fe2+ dosage) affecting this system were modeled by two approaches; Response Surface Method (RSM) and Artificial Neural Network (ANN). Although RSM has an acceptable prediction performance (R2pred = 0.87–0.92), and the models are well fitted (R2 = 0.95–0.96), ANN can deliver a more precise estimate of the experimental targets (53% and 79% less root mean square error for COD and ammonia removals, respectively). The modeling results confirmed that ANN could be trained satisfactorily using data obtained from the CCD experimental design. Sensitivity analysis emphasized the importance of pH and PMS/Fe2+ mass ratio in COD removal and the significant influence of pH on ammonia removal. Multi-objective optimization and experimental results at optimal conditions confirmed that maximum COD and ammonia removal with minimum catalyst consumption are 80.8% and 25.6%, respectively. The results show that hybrid activation of PMS can remarkably enhance the removal of refractory organic matters in landfill leachate compared to the previously studied SR-AOP systems. FTIR spectra results indicate that after 60 min of treatment by UV/PMS/Fe2+ process, the carbonyl groups disappeared, and the amount of C-O-C in aliphatic ethers increased due to chemical oxidation. In addition, the transmittance of the bands corresponding to aromatic CC and asymmetric stretch of COO- decreased significantly, suggesting that the degree of leachate humification has changed. The BOD/COD ratio of the final effluent improved from 0.52 to 0.99, meaning that the treated leachate has higher capability to be treated via biological methods.

- **Keywords:** SR-AOP; Modeling; Artificial neural networks; Response surface methodology; Peroxymonosulfate (PMS)

Yu Hu, Zhen Meng, YanZhu Hu, WenJia Tian, YanYing Yang, ShunLi Gao. *Modelling of accident dynamic spreading based on spike timing dependent plasticity*. Pages 727-739.

A large number of work safety accidents have exposed that accident has Domino Effect or Avalanche Effect: the chain reaction in system will be triggered when one critical node in system is disturbed, which will finally have an impact on large parts of the system. Exploring the interrelationships of elements on accident chain is very essential for studying the blocked mechanism of the accident. An improved model of dynamic of accident spreading in networks is proposed after analysing Complex Network theory and STDP mechanism. The model has the ability of independent learning of network edge

weight, and finally achieves the purpose of strengthening causality and weakening non-causality. We can abstract three kinds of ideal structure networks from a large number of realistic work safety accidents: the random networks, the scale-free networks and small-word networks. This model is simulated and analysed on the three networks, respectively. The process of time dynamic evolution of accident spreading and edge weight is analysed. The simulation results are consistent with the characteristic of actual work safety accident, which indicate that the model can effectively simulate the process of accident spreading dynamics of actual work safety accident and the process of edge weights evolution.

- **Keywords:** Work safety accident; STDP mechanism; Edge weight; Accident spreading; Time evolution

Zhixin Jin, Tao Huang, Xueming Zhang, Shaohui Zhang. *Bioelectrochemical-assisted bioleaching of chalcopyrite: Effect of pulp density, anode material, and sliver ion*. Pages 740-748.

Chalcopyrite bioleaching has developed rapidly because of the advantages such as environmental protection, low capital investment and simple operation, but its application has been limited by the slow reaction rate and other problems. Bioelectrochemical system (BES) as a promising wastewater treatment technology could solve the problem of reaction abort due to insufficient electron acceptors inside the mineral heap. In this study, the effect of pulp density, anode material and silver ion on the copper bioleaching were carried out. Experimental results showed that the maximum bioleaching efficiency (1.70 ± 0.18%) in 11 d was achieved at a pulp density of 1% with the application of titanium-silver anode and the assistance of BES. BES promoted the bioleaching of Cu mainly by promoting the bacterial reproduction and the Fe2+ production from the chalcopyrite. Moreover, the introduction of BES promoted the release of Ag+, further enhancing the bioleaching of Cu by 1.5 times (187.7 ± 18.1 mg/L vs. 120.9 ± 22.2 mg/L). In addition, the inhibition of conductive silver glue on the copper bioleaching and bacteria was alleviated by the BES. As an anode material, carbon cloth couldn't improve the leaching of Cu as compared to titanium foam, but it could increase the electron transfer efficiency.

- **Keywords:** Bioelectrochemical system; Chalcopyrite; Bioleaching; Copper extraction

Hadis Moteshafi, Leila Jabbari, Maryam Hashemi. *Performance of Bacillus subtilis D3d xylanase separated through optimized aqueous two-phase system in bio-bleaching of sugar beet pulp*. Pages 749-756.

Aqueous two-phase systems (ATPS) are potent, biocompatible, and cost-effective techniques for partitioning, concentration, or purification of biomolecules. In this work, the direct recovery of Bacillus subtilis D3d xylanase from the fermentation broth by the polymer-salt ATPS was optimized using response surface methodology (RSM). The 96% of xylanase recovery in the polyethylene glycol phase with the maximum purification factor (2.17 ± 0.02) and partition coefficient (69.87 ± 2.10) were the optimum responses that obtained at 9.5% (w/w) of polyethylene glycol, 20% (w/w) of sodium citrate, and pH 10. A good agreement between experimental and predicted results verified the adequacy of the RSM models. Furthermore, the efficiency of the crude and ATPS-recovered enzyme were evaluated in the biobleaching of sugar beet pulp. The ATPS-recovered enzymatic treatment of sugar beet pulp resulted in a higher release of reducing sugars (10.29 and 21.83 mg g−1) and caused 4.5% and 10% reduction in kappa number over crude-enzyme and control, respectively. This study indicated that ATPS-recovered xylanase compared to the crude enzyme has a promising application in the pulp and paper industry.

- **Keywords:** Xylanase; Aqueous two-phase system; Response surface methodology; Biobleaching; Sugar beet pulp

André Zamith Selvaggio, Felipe Matheus Mota Sousa, Flávio Vasconcelos da Silva, Sávio S.V. Vianna. *Application of long short-term memory recurrent neural networks for localisation of leak source using 3D computational fluid dynamics*. Pages 757-767.

Gas leaks represent a major concern in industrial sites due to potential human and economical losses. Prompt identification of leak scenarios favours corrective maintenance avoiding the domino effect. In this paper, long short-term memory recurrent neural networks were trained and tested to CH4 leakage source in a chemical process module. We exploit the benefits of varying the temporal length of input variables, and the datasets were obtained employing 3D-CFD simulations. We consider four leak locations, four wind speeds, and eight wind directions, besides the non-leakage scenario for the same wind speeds and directions. The models were trained using different values of timesteps to evaluate the prediction accuracy for unseen data. Results showed progressive improvement of the performance of the models with greater values of timesteps, and good generalisation with test accuracy over 95.3%, indicating the ability of the model to correctly predict the leakage source using easily monitored variables.

- **Keywords:** Methane release; Source localization; Process safety; Recurrent neural networks; Long short-term memory

Jianhao Yu, Jiahuan Yi, Haroun Mahgerefteh. *Optimal emergency shutdown valve configuration for pressurised pipelines*. Pages 768-778.

This paper presents the development and testing of a multi-objective optimisation technique for selecting the optimal in-line Emergency Shutdown Valve (ESDV) configurations for high-pressure transport pipelines. Using a real 150.2 km long, 1016 mm i.d. natural gas pipeline operating at 80 bar and 307.24 K as a case study, the optimisation technique is employed to strike the optimal balance between risk reduction, valve failure rate and capital cost expenditure. Starting with defining a set of six important valve and pipeline design characteristics as optimisation variables, Principal Component Analysis is employed to reduce the number of these parameters to three, reducing computational workload, whilst retaining accuracy. The results obtained using the multi-objective optimisation model are presented using scatter plots providing a geometrical visualisation of the set of optimal solutions in the space of objective functions. The findings demonstrate the efficacy of the proposed technique as an effective tool for the decision makers to select the optimal inline ESDV configurations, taking account of the valve type, pipeline overall dimensions, operating conditions, and the fluid composition being transported.

- **Keywords:** High-pressure pipeline safety; Emergency shutdown valve closure modelling; Multi-objective optimisation; Principal component analysis

Zongqi Zhang, Fangling Ruan, Siquan Xu, Wenting Wu, Shengbin Shi, Guomin Xiao. *Pervaporation separation of N, N-dimethylformamide/water using poly (vinyl alcohol) based mixed matrix membranes*. Pages 779-794.

Pervaporation is a separation technique relying on the concentration gradient, often expressed as partial vapor pressures, across polymeric or polymer-composite membranes. Those membranes inevitably exhibit a strong trade-off bottleneck between permeability and selectivity of target compounds, making the search for alternative materials with advanced performance characteristics highly desirable. This work aims to

incorporate the advance of polymer and inorganic fillers to synthesize mixed matrix membranes. Effect of inorganic filler on properties and separation performance of Poly (vinyl alcohol) based mixed matrix membranes was investigated extensively in terms of several means of characterization methods. The results showed that the addition of inorganic fillers, NaA, SBA-15, SiO2 and SiO2-NH2 not only enhanced the separation factor but also increased the flux of water and DMF resulting in advance in total flux. This study may provide a guide to separate DMF-water solutions and will contribute to expand the high-value utilization of mixed matrix membranes in pervaporation.

- **Keywords:** Pervaporation; Mixed matrix membranes; N, N-dimethylformamide/water (DMF/H2O) binary mixture; PVA and PVA membranes

Chao Wang, Yu Zhuang, Yutao Qin, Yachao Dong, Linlin Liu, Lei Zhang, Jian Du. *Design and eco-efficiency analysis of sustainable extractive distillation process combining preconcentration and solvent recovery functions for separating the tetrahydrofuran/ethanol/water ternary multi-azeotropic mixture*. Pages 795-808.

It is of great significance to design a sustainable extractive distillation separation configuration that can implement efficient separation of the ternary multi-azeotropic mixtures with a large single component content and propose a feasible and accuracy sustainable evaluation method. This is because the extractive distillation separation scheme with preconcentration should be designed for the particularity of such ternary multi-azeotropic azeotropes. To fill this gap, the paper designs a novel and sustainable three-column extractive distillation process containing one integrated distillation column (TCED-IDC) with both preconcentration and solvent recovery functions and two extractive distillation columns taking the separation of the tetrahydrofuran/ethanol/water ternary multi-azeotropic mixtures containing large amounts of water as an example. Simultaneously, economic optimization of the TCED-IDC process as well as the conventional three-column extractive distillation (TCED) process and the four-column extractive distillation (FCED) process is implemented to determine economically optimal design parameters via minimizing the total annual costs (TAC) using genetic algorithm. Following that, environmental and thermodynamic evaluations are comprehensively conducted to prove the advantages of the TCED-IDC process. The TCED-IDC separation schemes achieves 79.05%/8.47% reduction in CO2 emissions and 71.92%/9.57% economic cost savings compared to the TCED and the FCED schemes, and the corresponding thermodynamic efficiency is 7.87%. Moreover, an extended Eco-efficiency Comparison Index (ECI) method is proposed to perform the eco-efficiency analysis covering economic, environmental, and thermodynamic aspects for the three extractive distillation separation processes proposed. The analysis results demonstrate that the integration of preconcentration and solvent recovery functions improve the eco-efficiency compared to the other two separation schemes, and the corresponding ECI reaches 91.57% and achieves 1.42% points increase compared to the FCED scheme.

- **Keywords:** Extractive distillation; Integration of preconcentration and solvent recovery; Sustainability; Eco-efficiency analysis; Ternary multi-azeotropic mixture

Ganyu Zhu, Ziheng Meng, Shaopeng Li, Liwen Zhao, Fang Qi, Zhanbing Li, Shan He, Huiquan Li. *High efficiency desulfurization behavior by the sustainable low carbon utilization of carbide slag*. Pages 809-818.

For the purpose of the gradual decrease of calcium carbonate resources and reduction of carbon emissions in wet flue gas desulfurization process, the utilization process of carbide slag to replace limestone is systematically analyzed. The properties of carbide slag and limestone have been analyzed, and the mass transfer and reaction behaviors in desulfurization process have been calculated and comprehensively evaluated.

Desulfurization performances have been also compared through response surface analysis method. The results show that the calcium content and specific surface area of carbide slag are higher than limestone, which is conducive to the dissolution and mass transfer rate. Therefore, carbide slag is suitable for the treatment of flue gas with high SO2 concentration. Desulfurization efficiencies of the two desulfurization agents of carbide slag and limestone under the optimal process are 99.15% and 96.53%, respectively. In conclusion, carbide slag can be used in desulfurization process to replace limestone. The consumption of carbide slag slurry in the desulfurization process is about half of limestone slurry at the same conditions, and the higher desulfurization efficiency of carbide slag is attributed to the higher mass transfer and dissolution rate. Utilization of carbide slag also reduces the carbon emission in desulfurization process and economic cost. The reduction amount of CO2 emission can reach to about 0.76 t /t carbide slag. This work provides a basis for the industrial application and desulfurization efficiency improvement of carbide slag as the desulfurizer.

- **Keywords:** Carbide slag; Desulfurization; Mass transfer; Response surface methodology; Carbon emission reduction

Guangwei Wu, Luomei Zou, Fuyang Huang, Bin Wang, Sha Huang, Xia Shen, Shu Chen, Jingping Zhu. *Effect of humic substances derived from pastoral areas in Zoige Plateau on photodegradation of sulfamethoxazole and ciprofloxacin*. Pages 819-829.

Sulfonamides and quinolones are widely used antibiotics. Some end up discharged into aqueous environments where they can seriously affect human health and safety. The photochemical degradation of sulfamethoxazole and ciprofloxacin with the various concentrations was analyzed in different pH natural waters. Meanwhile, the effect of natural humic and fulvic acids on the photodegradation was tracked. The photolysis curves were perfectly consistent with the first-order kinetics. High concentration of antibiotics was not conducive to photodegradation. Photodegradation of ciprofloxacin was generally occur in neutral and alkaline environments, while photodegradation of sulfamethoxazole was generally in lower acidic environments. Persistent free radicals including reactive oxygen species were found in the photolytic reactions. They were found to arise both from auto-decay of the antibiotics and from decay of the humic substances. According to EPR test,·OH and 1O2 both have a good promotion effect on the photodegradation of antibiotics, and the contribution rate of 1O2 (50.63%) is greater than that of •OH (25.56%), indicating that 1O2 is the main active species in the photodegradation of sulfamethoxazole and ciprofloxacin, and the contribution rate of 1O2 produced by humic acids to the photodegradation of antibiotics is greater than that of fulvic acids. Humic substances produced a strong single signal with good symmetry in darkness and light, indicating that the free radicals produced by humic substances were EPFRs with stability and persistence. However, the amount of EPFRs produced by humic acids were more than that of fulvic acids, indicating that the free radicals produced by humic acids were the carbon center free radicals containing oxygen functional groups. Results of this study will provide further comprehensive fundamental data for risk assessment and control of antibiotics in farmland ecosystems in pastoral areas of Zoige Plateau.

- **Keywords:** Sulfamethoxazole; Ciprofloxacin; Fulvic acids; Humic acids; Photodegradation; Antibiotic waste

Xiangbao Meng, Yang Liu, Junfeng Wang, Zheng Wang, Ke Yan. *Experimental study and kinetic analysis on the deflagration characteristics of oil shale dust*. Pages 830-841.

In order to study the flame propagation characteristics and explosive overpressure characteristics of oil shale dust, the flame propagation and explosion characteristics of oil shale dust samples from two different regions (Longkou oil shale LKOS and Huadian oil shale HDOS) were tested by Hartman experimental device and 20 L spherical explosion experimental device respectively. The flame propagation velocity and brightness, the maximum explosion pressure (Pmax) and the maximum pressure rise rate ((dP/dt) max) obtained by experiments were analyzed. The research shows that the flame of oil shale dust develops slowly at the initial stage of explosion, and the propagation speed gradually increases with the development of the flame. The explosive flame of LKOS dust is brighter and fuller than that of HDOS dust with the same particle size, and has a faster propagation speed and stronger explosive. The Pmax and (dP/dt)max of LKOS dust are larger than HDOS dust. With the increase of dust mass concentration, the Pmax and (dP/dt)max of both show a trend of first increasing and then decreasing. The distributed activation energy model (DAEM) is used to calculate and analyze the pyrolysis volatiles release kinetic behavior of oil shale dust. The results show that the pyrolysis volatile analysis of LKOS has a higher rate of pyrolysis and volatilization, and the volatile gas is released faster during the explosion reaction. Which makes the explosive combustion reaction stronger.

- **Keywords:** Oil shale; Flame propagation; Explosion overpressure; Dynamic analysis

Xiaodong Lv, Kun Song, Yuntao Xin, Xuewei Lv. *Novel process for deep removal of chlorine and recycling of chlorinated tailings from titanium-bearing blast-furnace slag*. Pages 842-849.

Given the high chloride ion content in chlorinated tailings that harm the surrounding environment cannot be directly utilized, a new process for the deep removal of chloride ions from chlorinated tailings with additives was proposed. The products obtained included tailing slag, which can be used as a building material, and salt, which can be used in industry. Theoretical calculations and experiments were performed to determine the feasibility of the new process. The results showed that the chloride ions from the chlorinated tailings and sodium ions from the additives formed NaCl, which could be removed during water leaching. NaOH served as a better additive than sodium sulfate. An increase in the molar ratio and the prolongation of ball-milling was beneficial for the dechlorination of the water leaching residue. An increase in the roasting temperature leads to an increase in particle size, which worsens the kinetics of subsequent leaching and reduces the leaching rate. The developed process can obtain tailings with chloride ion content of less than 0.1%, which meets the standard for building materials applications. Meanwhile, NaCl with a purity greater than 99% could be obtained, preventing chloride ion pollution of water resources and the comprehensive utilization of chlorinated tailing.

- **Keywords:** Chlorinated tailing; Dechlorination; Alkaline transformation; Comprehensive utilization

Thor Alexis Sazon, Teruyuki Shimizu, Yasuhiro Fukushima, Tadafumi Adschiri, Yasunori Kikuchi. *Energy intensity in applying low-temperature chemical looping in steam reforming*. Pages 850-861.

An energy analysis of methanol production via low-temperature chemical looping steam reforming was performed based on the process design; the potential benefits in reducing fuel consumption and excess heat generation were analysed. The feasibility of performing chemical looping reforming at temperatures lower than the conventional 900 °C is linked with the on-going development of a suitable oxygen carrier through the supercritical method. Pinch analyses were performed on designs that operate at three different reforming temperatures, namely 900, 500, and 300 °C, with either a high or a low heat

transfer assumption within the reforming furnace. The results show that notable benefits are expected if the heat transfer from the combustion gases to the reformer tube contents improves along with lowering the reforming temperature. This 'optimistic scenario' resulted in an ≈ 41% decrease in excess heat generation and an ≈ 55% decrease in fuel consumption, as the reforming temperature decreased from 900° to 300°C. However, in the 'pessimistic scenario', where heat transfer does not improve despite the reforming temperature lowering, fuel consumption and excess heat generation remained almost constant when the reforming temperature was lowered from 900° to 300°C. In reality, heat transfer within the reforming furnace could behave somewhere between the low and high heat-transfer assumptions. The benefits of lowering the reforming temperature thus depend on several process and equipment design factors, including the temperature driving force, heat transfer area, and pinch approach temperature. An ill-designed reforming furnace, represented by the low heat-transfer scenarios, could result in no significant improvements despite the lowering of the reforming temperature; whereas well-designed equipment, represented by the high heat-transfer scenarios, could bring a significant improvement in energy consumption and waste heat generation.

- **Keywords:** Chemical looping; Steam methane reforming; Methanol synthesis; Pinch analysis; Heating and cooling duty

Gandharve Kumar, Raj Kumar Dutta. *Sunlight mediated photo-Fenton degradation of tetracycline antibiotic and methylene blue dye in aqueous medium using FeWO4/Bi2MoO6 nanocomposite*. Pages 862-873.

An optimized batch of 0.25FeWO4/Bi2MoO6 nanocomposites has been developed as an efficient solar photo-Fenton catalyst for degradation of tetracycline antibiotic and methylene blue in an aqueous medium. The catalyst is synthesized by hydrothermal route. Its structure, composition, and morphology are thoroughly characterized. The catalyst dose of 30 mg/50 mL spiked with 20 µL of H2O2 (30% v/v) resulted in 97% degradation of tetracycline and 99% degradation of methylene blue within 90 min. The corresponding degradation rate constants are 0.026 min−1 and 0.043 min−1, respectively. The total organic carbon estimation indicated mineralization of ~80% tetracycline and ~90% methylene blue. The photo-Fenton degradation of tetracycline and methylene blue by FeWO4/Bi2MoO6 nanocomposites is significantly enhanced as compared to Bi2MoO6 photocatalyst, attributed to photo-Fenton heterojunction catalyst, charge carrier separation and mobility, and sustained reactive oxygen species (ROS) generation. The role of ROS, e.g., hydroxyl radicals and superoxide radicals, towards the degradation process is confirmed from ROS scavenging studies. The degradation mechanism has been discussed by identifying the degradation products by ultra-performance liquid chromatography (UPLC)-Q-Tof-MS technique.

- **Keywords:** FeWO4/Bi2MoO6 nanocomposite; Solar photo-Fenton degradation; Degradation kinetics; Degradation product analysis; Reactive oxygen species

Hasan Ali Mahdieh, Nasser Talebbeydokhti, Seyed Hosein Afzali, Ayoub Karimi-Jashni. *Development and evaluation of a novel feed spacer for forward osmosis membrane*. Pages 874-886.

This paper introduces new feed spacer geometry for the forward osmosis (FO) membrane modules in an attempt to achieve more water flux than conventional models. The geometry is based on a mesh with star-shaped cross-section filaments, and it is optimized by using the response surface methodology (RSM) with a central composite design (CCD) in a series of numerical simulations. Filament thickness, filaments distance, and curvature radius are evaluated as main geometry parameters, while pressure drop and water flux are observed as responses. Two models are extracted with R2 of more than 99%. Results show the filament thickness and distance have a highly significant

effect on responses. Simultaneous optimization of water flux and pressure drop predict the best results would be obtained with a filament thickness of 0.4 mm, a filament distance of 2.32 mm, and a curvature radius ratio of 0.7 with a desirability of 0.66. The vertical movement of filaments in the channel, zigzag, and uniform mode, negatively affect the spacer performance. The results of the newly developed spacer were compared with those of a commercial spacer with 31 mil thickness. The optimized spacer achieved 8% more water flux than the commercial 31-mil spacer in the proposed conditions. This research shows that the newly developed FO spacers could improve the performance of this process.

- **Keywords:** CFD; Forward osmosis; Spacer; Optimization; RSM

Peng Gao, Weijun Li, Yibo Sun, Shuanglei Liu. *Risk assessment for gas transmission station based on cloud model based multilevel Bayesian network from the perspective of multi-flow intersecting theory*. Pages 887-898.

Accidents occurred in the natural gas transmission stations may result in casualties, equipment damage, property loss and even political and ecological impact. It is necessary to propose an approach for the gas transmission stations risk assessment so as to identify risk factors and prevent accidents. However, insufficient attention has been paid to the complex interactions and coupling patterns of these factors with current risk assessment methods. Hence, a novel risk analysis strategy is needed for industrial site risk assessment. Given industrial site risk factors, the multi-flow intersecting theory (MIT) is first defined to consider material, information and behavior risk analysis. Then the multilevel Bayesian network is constructed to represent these factors from different flows. To handle issues of insufficient statistical data and subjectivity associated with expert judgement, cloud model and fuzzy Bayesian are incorporated. For the defuzzification, existing cloud model is improved by introducing the similarity degree of standard cloud and evaluation cloud. Then the prior and conditional probabilities obtained from cloud model are input into Bayesian network for further reasoning and accident probability prediction. To validate the utility of the proposed method, the gas transmission startup process was chosen for risk assessment.

- **Keywords:** Gas transmission station; Risk assessment; Multilevel Bayesian network; Multi-flow intersecting theory; Cloud model

Kazuko Yui, Hidetoshi Kuramochi, Masahiro Osako. *Measurement and modeling of heavy metal behaviors during the incineration of RDF in a pilot-scale kiln incinerator–Part 2: Incineration test*. Pages 899-910.

This paper is part of the studies that examine the performance of multizonal thermodynamic equilibrium calculation applied to waste incineration, and the primary objective was to obtain experimental data on the fate of elements in a waste incinerator under a controlled condition for comparison with the results of the calculation. We conducted an incineration test of refuse dried fuel (RDF) made from municipal solid waste (MSW) using a pilot-scale kiln incinerator, which enables us to control the combustion condition and reduce the fluctuation of the waste composition during the incineration test. The second objective was to obtain the fundamental characteristics of RDF incineration residues, as there was limited information about RDF incineration in the literature. The incineration residues obtained had uniform appearance, and the recovery ratios of total ash and individual elements were around 100%, which is suitable for use in the checking of the performance of the calculations. The elemental and mineralogical composition of the RDF incineration residues was analyzed. The fate of elements in the RDF incinerations was similar to those of ordinary MSW incinerations in the literature,

whereas the RDF ash contained more Ca-rich minerals than MSW, reflecting the composition of the RDF.

- **Keywords:** RDF; Municipal solid waste; Incineration; Heavy metal; XRD; SEM-EDS

Singamsetty Harikrishna, Kranthi Kumar Gangu, Alice R. Robert, Himavathi Ganja, Nagaraju Kerru, Suresh Maddila, Sreekantha B. Jonnalagadda. *An ecofriendly and reusable catalyst RuO2/MWCNT in the green synthesis of sulfonyl-quinolines*. Pages 911-917.

A simple and efficient RuO2/MWCNT nanocatalyst has been synthesized and thoroughly characterized by powdered XRD, SEM, SEM-EDX, TEM, and N2 adsorption analysis. The catalytic activity of RuO2/MWCNT nanomaterial was investigated in the effective green synthesis of sulfonyl-quinoline derivatives (5a–j) in higher yields applying a one-pot four-component reactions of substituted aldehydes, dimedone, phenylsulfonyl acetonitrile and NH4OAc in ethanol. The conversion was high under optimal conditions. The catalyst material could be separated easily from the reaction mixture and recyclable eight times via simple filtration without considerable reduction of its catalytic efficiency. Simple handling, eco-friendly, inexpensive, excellent yields (91–98%), minimum reaction time (≤15 min), use of green solvent and easy work-up are the features of this methodology.

- **Keywords:** Green Synthesis; Heterogeneous catalysts; RuO2/MWCNT; Sulfonyl-quinolines; Multi-component reaction; One-pot synthesis

Juan Gabriel Segovia Hernández, Fernando Israel Gómez-Castro, Araceli Guadalupe Romero-Izquierdo, Carolina Conde-Mejía, Antioco López-Molina. *Partial energy integration between biofuels production processes: Effect on costs, CO2 emissions and process safety*. Pages 918-930.

Energy integration is a tool which allows reducing the heating and cooling requirements for production processes. This is particularly important in the processes for production of biofuels, since such processes are expected to have low environmental impact, which can be achieved by reducing the need for steam and cooling water. It is common to perform energy integration by making use of all the available streams. This approach may allow reducing as much as possible utilities' requirements, but other indicators may be affected, such as capital costs, since the number of required equipment is increased. Thus, in this work the effect of performing partial integration is assessed, i.e., selecting only a few streams to perform the energy integration. The effect of increasing the number of integrated streams is assessed in terms of sustainability indicators based on the green chemistry principles. The studied indicators are utilities' requirements, total annual cost, environmental impact (assessed through CO2 emissions) and safety (assessed through the HPSI index). The study is applied to the energy integration of a supercritical biodiesel production process and a lignocellulosic bioethanol production process.

- **Keywords:** Energy integration; Partial integration; Biofuels; Economic assessment; Sustainability; Risk assessment

Yunshu Zhang, Jing Ding, Qingwei Gao, Bo Jiang, Cong Li, Qingliang Zhao. *Synthesis of low-cost Ti4O7 membrane electrode for electrooxidation of tetracycline under flow-through conditions: Performance, kinetics and mechanism*. Pages 931-943.

The high cost of anode material and the limitation of liquid-mass transfer on anode surface in electrochemical advanced oxidation processes always restrict the removal efficiency of organics. To overcome the limitations, this study synthesized a low-cost Ti4O7 membrane electrode by simple sol-gel method, and developed a flow-through electrooxidation system based on Ti4O7 membrane electrode. The membrane electrode presented high crystallinity, high specific surface area (10.18 m2/g), concentrated pore sizes distribution (0.1–1 μm), and high oxygen evolution potential (2.2 V vs. SHE). Furthermore, compared with stirring conditions, the flow-through conditions could enhance the liquid-mass transfer on anode surface, resulting in a high tetracycline degradation efficiency (97.24%) and a low energy consumption (0.18 kWh/gDOC). High degradation rates of tetracycline (more than 95%) were both observed with the initial tetracycline concentration ranged from 10 to 50 mg/L. The increase of pipeline pressure and current density had positive influence on tetracycline degradation. Hydroxyl radicals and sulfate radicals produced on the electrode surface are the main oxidants for tetracycline degradation. The degradation pathway of tetracycline included oxygenation, hydroxylation, demethylation, decarbonylation, ring-open, and C-N bond cleavage. Compared with materials prepared by conventional hot pressing and plasma spraying method, this simply synthesized Ti4O7 membrane electrode exhibited efficient oxidation capability and competitive electric cost for contaminants degradation, demonstrating its practicability, feasibility, and facilitation for the potential application.

- **Keywords:** Electrochemical advanced oxidation processes; Ti4O7 membrane electrode; Sol-gel method; Flow-through; Tetracycline

Qingcheng Hu, Jianguang Yang, Tianxiang Nan, Xuezhen Xie, Youming Ye. *Study on the electrically enhanced process for cadmium removal by a pulse in a sulfuric acid system*. Pages 944-952.

Aiming at the problems of low cadmium removal efficiency in zinc replacement and poor pressing plate effect of cadmium residues in the latter stage of the process, a novel electrically enhanced replacement method for cadmium removal based on a pulsed electric field was proposed. Comparative experiments with different current types verified the superiority of pulse current in the cadmium removal process to other known methods. At 45 °C, anode current density of 20 A·m−2, cathode-to-anode area ratio of 1:3, pulse duty ratio of 1:4, and pulse frequency of 500 Hz, the cadmium removal efficiency reached 96.80% in three hours. Furthermore, electrochemical test results for anodic reaction illustrated that the rise in solution acidity and Cd2+ concentration accelerated the replacement of zinc to cadmium. Correspondingly, increases in temperature, Cd2+ concentration, and solution pH inhibited the dissolution of the precipitated cadmium.

- **Keywords:** Cadmium treatment; Application of pulse; Electrical reinforcement; Anodic reaction mechanism

Diego Juela, Mayra Vera, Christian Cruzat, Ana Astudillo, Eulalia Vanegas. *A new approach for scaling up fixed-bed adsorption columns for aqueous systems: A case of antibiotic removal on natural adsorbent*. Pages 953-963.

The scaling up of adsorption columns is a crucial step toward the removal of emerging pollutants from domestic and industrial wastewaters. In this study, a fixed-bed column to remove sulfamethoxazole packed with sugarcane bagasse was scaled up from laboratory (DL = 2.2 cm) to pilot unit (DP = 4.4 cm) using a scaling factor (K = 2). In addition to the basic similarity rules for scaling, three new criteria were proposed for the mass adsorbent, flow rate, and bed volume. Then, three lab-scale tests at flow rate of 5 mL/min and bed heights of 15, 25, and 35 cm were transferred to the pilot-scale

column at flow rate of 20 mL/min and bed heights of 30, 50, and 70 cm, respectively. The breakthrough curves and the fixed-bed parameters (residence time tR, saturation time ts, adsorption capacity qe, volume of solution treated Vef, and removal percentage %R) obtained in both scales were compared to define their effect with the increase of scale. Finally, a mechanistic model was proposed to predict the breakthrough curves in both columns. The results exhibited that the breakthrough curves in the pilot-scale prolonged in time with higher breakthrough and saturation times than the laboratory breakthrough data. Additionally, tR, ts, and Vef changed in function of the K value used: ts and tR doubled their value in the pilot column or tRP=KtRL; Vef was eight times higher in the pilot column than the lab-column or VefP=K3VefL; qe and %R remained constant in both scales; these results were corroborated with the predicted breakthrough curves. Besides, the mechanistic model predicted with great precision the breakthrough data in both scales (R2>0.9), which means that the model can be used confidently for scaling up purposes. This study demonstrated new criteria which can be easily applied to scale up adsorption columns whit results that showed a correlation between both scales.

- **Keywords:** Scaling up; Wastewater treatment; Antibiotic removal; Biosorption; Modeling

Xuexian Li, Hongyan Liu, Wei Meng, Nanting Liu, Pan Wu. *Accumulation and source apportionment of heavy metal(loid)s in agricultural soils based on GIS, SOM and PMF: A case study in superposition areas of geochemical anomalies and zinc smelting, Southwest China*. Pages 964-977.

Heavy metal(loid)s (HMs) in soils of Southwest China naturally have a high background and are superimposed with intensive anthropogenic activities, resulting in serious accumulation of HMs in regional agricultural soils, which poses threat to ecological security and agricultural product quality. The accumulation and source apportionment of HMs in agricultural soils are not only one of the focuses of global concern but also a challenging task worldwide. In the present study, a total of 395 topsoil samples (0–20 cm) and 19 deep soil samples (150–180 cm) were collected from typical artisanal zinc smelting regions in northwestern Guizhou Province, China to investigate the spatial distribution, accumulation and source apportionment of HMs (As, Cr, Cu, Hg, Ni, Pb, Cd and Zn) based on the combined approach of enrichment factor (EF), self-organizing map (SOM), geographical information system (GIS), and positive matrix factorization (PMF). The mean contents of As, Cr, Cu, Hg, Ni, Pb, Cd and Zn in agricultural soils all exceeded the corresponding local background values, and obvious enrichment of Cd was found in the studied topsoil, followed by Pb, Cu, and Zn. Combined with SOM and PMF analysis, five potential HMs sources were identified: Cd (74.58%), As (32.05%), Zn (30.57%), Hg (23.16%), and Pb (11.38%) were associated with artisanal Zn smelting activities; Cu (66.08%), Zn (18.12%), Ni (17.25%), Cd (16.95%), and Pb (10.08%) were mainly from agricultural activities; Pb (68.9%), Zn (25.73%), and As (22.64%) were mainly from traffic emissions and smelting-related activity sources; Hg (68.55%), As (45.31%), Cr (38.63%), and Ni (32.44%) were primarily from atmospheric deposition associated with industrial activities and coal combustion; and Cr (61.01%), Ni (44.52%), Zn (17.32%), Cu (16.11%), and Cd (8.39%) mainly originated from soil parent materials. The proportions of the five potential sources were 14.5%, 20.9%, 19.8%, 17.8%, and 27%, respectively. Anthropogenic sources accounted for the largest contribution (approximately 73%) to the soil HMs, especially the artisanal zinc smelting activities to Cd, Zn, As, Hg, and Pb, which was significantly higher than that of geological sources, suggesting that intense human activities produced a large amount of HMs enrichment in topsoil. The SOM clustering and source apportionment of soil HMs are of great significance for reducing HMs pollution sources, and can provide scientific guidance for pollution prevention and regional remediation of HMs in agricultural soils.

- **Keywords:** Soil heavy metal(loid)s; Accumulation assessment; Source apportionment; SOM; PMF

R.A. Gado. *The feasibility of recycling marble & granite sludge in the polymer-modified cementitious mortars Part A: In polymer-modified cementitious adhesive mortar*. Pages 978-991.

In the present scientific article, a potential assessment and feasibility study of the recycling process of marble and granite sludge into the system of pre-packed polymer-modified cementitious mortar products has been investigated instead of being disposed of or landfilled. Therefore, several polymer-modified mortar formulations were designed to explore the inclusion effect of marble and granite sludge waste on the overall performance of the prepared mortar formulations in the application area of the polymer-modified cementitious adhesive. In this work, starting raw materials and hardened mortar specimens (28 days) of the prepared mortar formulations were well-characterized by different scientific techniques, including X-ray fluorescence for chemical oxides composition, X-ray diffraction for mineral phases composition Fourier-transform infrared (FTIR). To achieve the study's goals, different percentages of marble and granite sludge were incorporated into the prepared mortar formulations in the range of 0%, 5%, 10%, 15%, 20%, 25%, and 30% to replace the used silica sand in each formulation. The results showed that the marble and granite sludge waste is mainly composed of calcite and quartz minerals, with an average particle size of 4.86 μm. The results also showed an improvement in the workability, performance, and adhesion strength of the prepared polymer-modified cementitious adhesive mortar formulation upon using the optimum sludge addition percentage. Moreover, the experimental results show that the compressive and flexural strength of the prepared mortar formulations were also enhanced by increasing the sludge content.

- **Keywords:** Polymer-modified mortar; Cementitious adhesive; Marble & granite sludge; Reuse and recycle

Shuang-Hua Yang, Jian-Meng Chen. *Air pollution prevention and pollution source identification of chemical industrial parks*. Pages 992-995.

This special issue aims to provide innovative research work that has recently been carried out in air pollution prevention and pollution source identification of chemical industrial parks, including both theoretical developments, experimental and/or application research. Chemical industrial parks have become a critical production space and brought enormous economic benefits to the regions. Consequently, they have caused tremendous pressure on the surrounding and regional environment. This preface firstly introduces the features of chemical industrial parks, then presents the five challenges on air pollution prevention, pollution source identification and source term estimation, and finally summaries the thirteen papers included in the special issue.

Jaydev Kumar Mahato, S.K. Gupta. *Advanced oxidation of Trihalomethane (THMs) precursors and season-wise multi-pathway human carcinogenic risk assessment in Indian drinking water supplies*. Pages 996-1007.

Advanced oxidation processes (AOPs) in water treatment industries can simultaneously offer disinfection and eradicate organic contaminants. The present work examined the direct exposure impact of various oxidative (UV, O3, and H2O2) and their eclectic combinations (UV/O3, H2O2/O3, and UV/H2O2) for the abolition of Trihalomethane (THMs) precursors. The application of the Fenton process proved to be the most effective technique for reducing TOC (85.23%) and UV254 (91.11%) than other used AOPs.

Higher removal of THMs precursors found in the Fenton process may be attributed to the higher degradation potential of hydroxyl radical generated from this process than other AOPs. The deformed ferrous iron salts (Fe2+) in the Fenton reagent catalyzed the hydrogen peroxide (H2O2) and produced highly reactive radicals. Seasonal probabilistic lifetime cancer and non-cancer risks of THMs in males and females were also investigated in the drinking water supplies of five major cities in India. Comparative risk analysis through different pathways revealed significant risk from oral ingestion (99%), followed by inhalation exposure (0.77%) and dermal absorption (0.002%), where females were found at higher risk of cancer. Sensitivity analysis using a radar plot was also performed to identify the most influential parameter affecting the total risk of cancer. The Risk value of chloroform (CF) was highest among the THMs compound in all the WTPs for both seasons. Seasonal risk assessment revealed a higher risk of cancer in the pre-monsoon season.

- **Keywords:** Drinking water; Advance oxidation process; NOM; THMs health risk; Sensitivity analysis

Juan F. Saldarriaga, Ximena Gaviria, Jorge M. Gene, Roberto Aguado. *Improving circular economy by assessing the use of fly ash as a replacement of lime pastes reducing its environmental impact*. Pages 1008-1018.

In this work, bituminous coal, sugar cane, untreated and pretreated hazardous waste ashes are tested as supplementary cement materials, analyzing their reactivity in lime pastes prepared according to ASTM C–305, using a 0.5 water/lime ratio. The hydration process was stopped with acetone at the ages of 1, 3, 7, 14, 28, 56, 90 and 180 d. Mineral phases were determined by thermogravimetry, XRD, and SEM finding high contents of SiO2 and Al2O3 in the coal and sugarcane ashes, while in the hazardous waste ashes low contents of these oxides were found. Samples of sugarcane and untreated hazardous waste ashes seems to be attractive to be used as substitutes in the production of construction supplies. In addition to this, an E-factor analysis was carried out, which showed that carrying out fly ash replacements in any quantity contributes to the circular economy of all the economic activities involved. Reducing the amount of solid waste to be disposed of and improving the local and regional environmental quality.

- **Keywords:** Fly ashes; Lime paste; Reactivity; Waste; Circular economy

Seyed Ali Mousavi, Mehdi Mehrpooya, Mostafa Delpisheh. *Development and life cycle assessment of a novel solar-based cogeneration configuration comprised of diffusion-absorption refrigeration and organic Rankine cycle in remote areas*. Pages 1019-1038.

The increasing power demand in the world's energy basket and the focus on reducing carbon emission, in tandem with upgrade constraints on conventional grids, has elicited the employment of renewable energies. Specifically, answering the power and cooling/heating demands of remote areas where the grid cannot or can merely supports using locally available and utilizable renewable energies is a focal topic. Herein, a cogeneration system driven by solar energy through parabolic trough collector (PTC) utilization integrated with organic Rankine cycle (ORC), and diffusion absorption refrigeration (DAR) cooling system is proposed. The system is backed up by phase-change material (PCM) and battery bank for solving the intermittence nature of solar energy, and targeted at being employed in a residential building in Shahr Asb, a village in Yazd province, Iran, with a population of less than 600. The system is appraised through exergy evaluation to gauge the efficiency and performance of the system, and life cycle assessment analyses (exergoenvironmental evaluation), to present beneficial data on the mutual impact of the system's performance and environmental conditions. The HYSYS,

MATLAB, TRNSYS, and HOMER software and programming environments were utilized to model the cogeneration system. The exergy analysis indicated that the PTC field contributed to the highest exergy destruction (31.80 kW) of the system (67.89 kW) with PTC and system exergy efficiency of 55.23% and 67.89%, respectively. Consistent with the exergoenvironmental analysis, the highest values of cumulative environmental impacts were pertinent to EX-101 expander, (204.02 Pts/h - 29.49%) and E-102 heat exchanger (154.44 Pts/h - 22.33%), individually. Consequently, to mitigate the system's undesirable environmental impacts, the operating conditions of these devices must be amended. The parametric analysis showed that the rise in mole fraction of hydrogen as the inert gas of the DAR system positively affects the evaporator duty and temperature. The required power (10.76 kW) and cooling (44.55 kW) are provisioned by utilizing 80.76 kW and 364.30 kW of heat duty in the DAR and ORC system, respectively, which is met by the battery bank and PCM when solar energy is absent during the night.

- **Keywords:** Hybrid energy system; Diffusion absorption refrigeration; Parabolic trough solar collector; Phase change material, Battery bank; Life Cycle Analysis

Yue Gao, Guozhi Cao, Litiao Hu, Jun Bi, Zongwei Ma. *Spatially resolved risk assessment of Natech in the Yangtze River Economic Belt, China*. Pages 1039-1052.

China is not only a large industrial country but also one of the countries with severe natural disasters in the world. The impact of a technical accident triggered by natural disasters (Natech) cannot be ignored. In Natech risk assessment, most research focuses on the quantitative analysis of Natech risk in small-scale level areas, such as parks or enterprises; Natech risk assessment in large-scale areas is typically at low resolution. There is a lack of systematic and high-resolution assessments on a large regional scale. In this paper, a grid Natech risk assessment method that couples the probability model and the information diffusion method is proposed. We select the Yangtze River Economic Belt (YREB) as the research area to assess its Natech risks triggered by floods, earthquakes and typhoons with a spatial resolution of 1 km × 1 km. The results show that the atmospheric risk level is higher than the water environment risk level, but their distribution trends are roughly similar. For the Natech risk triggered by floods, the high-risk areas of the atmosphere and water accounted for 3.83% and 1.73% of the YREB respectively, and were distributed along with the river network. For the Natech risk triggered by earthquakes, the high-risk areas of the atmosphere and water accounted for 0.47% and 0.08% of the YREB, respectively, and high-risk areas were mostly concentrated in north-central Sichuan and northern Yunnan. For the Natech risk triggered by typhoons, the high-risk areas of the atmosphere and water accounted for 3.52% and 2.68% of the YREB respectively, which were mostly concentrated in parts of Jiangxi and south-eastern Hunan. The spatially resolved map can help to identify the spatial characteristics and hot spots, which can provide a scientific reference for macro decision-making in environmental risk management.

- **Keywords:** Natech risk; Yangtze River Economic Belt; Spatially resolved assessment; Probability model; Information diffusion

M.F. Paucar-Sánchez, M. Calero, G. Blázquez, M.J. Muñoz-Batista, M.A. Martín-Lara. *Characterization of liquid fraction obtained from pyrolysis of post-consumer mixed plastic waste: A comparing between measured and calculated parameters*. Pages 1053-1063.

In this study, thermal pyrolysis of a real mixture of plastic wastes collected from municipal solid waste of Granada (Spain) was performed to obtain a liquid oil. The goals of the present study were: 1) identify the optimal conditions to obtain maximum yields of the liquid fraction, 2) experimentally measure basic characteristic parameters of pyrolytic

oils, 3) use correlations or equations used in the hydrocarbon industry to estimate the measured properties, 4) make a comparison between the measured and calculated properties by predictive mathematical expressions, 5) develop new correlations for estimating pyrolytic oil properties. As main results, the optimal temperature to obtain maximum yield of liquid fraction was 500 °C. The physical and chemical properties of pyrolytic oils changed as temperature increased due to the presence of hydrogenation and dehydrogenation reactions. Also, the approximation of the chromatography data allowed to determine, by simulated distillation, the potential fuel yields that will be obtained if processed as synthetic crude in an atmospheric tower and a vacuum tower. Finally, two novel modified equations were proposed to estimate the specific gravity and refractive index parameter for pyrolytic oils.

- **Keywords:** Thermal cracking; Waste plastics; Pyrolysis; Hydrocarbons characterization

Ruichao Wei, Jiamei Lan, Liping Lian, Shenshi Huang, Chen Zhao, Zhurong Dong, Jingwen Weng. *A bibliometric study on research trends in hydrogen safety*. Pages 1064-1081.

Hydrogen plays an increasingly significant role in solving the greenhouse effect and energy crisis as a clean fuel that can be obtained by renewable energy, and as a storable energy carrier. As a prerequisite for process safety of hydrogen, issues such as hydrogen embrittlement, fire, and explosion, have been of great interest to research scholars for decades. Based on bibliometrics, this article aims to provide a knowledge structure of publications related to hydrogen safety. Information about 369, 535 and 462 publications related to hydrogen safety from 1957 to 2021 were retrieved from the Web of Science Core Collection, Scopus, and Lens, respectively. The visualization software VOSviewer was employed to carry out the bibliometric analysis. The study found that the USA has the most publications among all countries; the publications from the International Journal of Hydrogen Energy rank the first among all source journals. Based on the advancement of time period, the hot terms in hydrogen safety research can be divided into three themes: storage and detection, combustion and explosion, and ignition and propagation. The results provide a comprehensive overview of this field of research and can help researchers quickly understand the research frontier and the overall status.

- **Keywords:** Hydrogen safety; Bibliometric analysis; Knowledge structure; Visualisation

Sai Li, Tong Yue, Wei Sun, Chenyang Zhang, Jianyong He, Mingjun Han, Hongliang Zhang, Heng Yu, Wenyuan Li. *Intense removal of Ni (Ⅱ) chelated by EDTA from wastewater via Fe3+ replacement–chelating precipitation*. Pages 1082-1091.

Efficient removal of Ni (Ⅱ) chelated by ethylenediaminetetraacetic acid (EDTA) from wastewater remains an important but challenging environmental problem. Therefore, a novel strategy of Fe3+ replacement–chelating precipitation was proposed to remove Ni (Ⅱ) chelated by EDTA from simulated Ni-EDTA wastewater and real electroless nickel plating wastewater. The strategy was proved to be thermodynamically feasible by DFT calculation. Regardless of the simulated Ni-EDTA wastewater or the real electroless nickel plating wastewater, the residual nickel in the wastewater was less than 0.1 mg/L that satisfied the discharge standard after being treated under optimal conditions using this strategy. Moreover, the strong acidity and Fe3+ could increase the proportion of free Ni2+ in Ni-EDTA wastewater, thereby enhancing the Ni removal efficiency. Additionally, the total amount of EDTA in wastewater was basically unchanged, since the structure of EDTA was not destroyed by this strategy, while its chemical form changed from Ni-EDTA complex to Fe3+-EDTA complex. Furthermore, the mechanism was systematically

studied by electronic structure analysis, solution chemistry, UV-Vis spectral, FT-IR spectral and X-ray photoelectron spectroscopy. At last, this strategy is a promising approach and it can provide a reference for the treatment of other similar heavy metal wastewater.

- **Keywords:** Ni-EDTA complex; DFT; Wastewater treatment; Dithiocarbamates; Mechanism

Mainak Mukherjee, Sanjukta Roy, Krishanu Bhowmick, Swachchha Majumdar, Indah Prihatiningtyas, Bart Van der Bruggen, Priyanka Mondal. *Development of high performance pervaporation desalination membranes: A brief review*. Pages 1092-1104.

Water scarcity rises as the level of water pollution continues to increase with the progress of urbanization, industrialization and exponential growth of population. Therefore, saline water of the sea should also be made suitable rather than river water to meet the huge global demand of clean and safe drinking water. Pervaporation (PV) desalination, among many purification and separation processes, is a promising technology to reduce the crisis of global drinking water supply. From this perspective, the key success of PV desalination relies on its remarkable salt rejection from highly saline water with appropriate flux to obtain fresh water by using a suitable membrane. In this review we aim to provide a comprehensive assessment of PV desalination membrane materials, transport phenomena, the advantages of the process over comparable technologies (e.g., fractional distillation, membrane distillation, reverse osmosis) and the advantages of crosslinking during the preparation of composite membranes. This review further highlights the advantages of inorganic ceramic substrates as a support of composite membranes and the use of hydrophilic polymers as active layer for preparing stable and robust crosslinked PV desalination membranes.

- **Keywords:** Pervaporation; Desalination; Composite membrane; Ceramic; Crosslink

Jie Chen, Chao Zhu, Junsheng Du, Yuanyuan Pu, Pengzhi Pan, Jianbiao Bai, Qingxin Qi. *A quantitative pre-warning for coal burst hazardous zones in a deep coal mine based on the spatio-temporal forecast of microseismic events*. Pages 1105-1112.

The quantitative prediction for a coal burst is challenging since the coal burst mechanism is extremely complex with a verity of influencing factors involved. This study proposes a data-driven strategy to dynamically determine the coal burst hazardous zones in a deep coal mine based on quantitative predictions for microseismic events. A deep learning model, MSNet, comprising a convolutional module, a recurrent module, a skip-recurrent module, and an autoregressive module is built to predict the time, location, and energy for imminent microseismic events. More than ten thousand microseismic events from a workface were collected to form the database for the MSNet model training and testing. The results indicated that the MSNet can predict the event location accurately but that it predicts event timing less accurately. The MSNet demonstrated the worst prediction accuracy for event energy. Furthermore, this study analyzed the possible causes of the model's prediction errors and provided ways for enhancing the model's performance. Finally, a coal burst intelligent pre-warning platform was developed, which has been successfully used in coal mines at present. This study realized the quantitative forecast for coal burst hazardous areas on a preliminary basis while laying a foundation for coal burst timing risk prediction.

- **Keywords:** Coal burst; Deep learning; Microseismic event; Intelligent pre-warning platform

Danilo H.S. Santos, João P.T.S. Santos, José L.S. Duarte, Leonardo M.T.M. Oliveira, Josealdo Tonholo, Lucas Meili, Carmem L.P.S. Zanta. *Regeneration of activated carbon adsorbent by anodic and cathodic electrochemical process*. Pages 1150-1163.

The efficiency of saturated Activated Carbon (AC) electrochemical regeneration was evaluated. Reactor configurations in cathodic/anodic process, applied current effect on the properties of AC and Methylene Blue MB-AC interactions and adsorption/desorption mechanisms were studied. The efficiency was measured by adsorption capacity adsorption/regeneration cycles and changes in the adsorbent characteristic were analyzed through FTIR, BET, Optical Microscopy (OM) and SEM before and after the regeneration. The energy consumption was analyzed to assess the economic feasibility. It was found that the electrochemical treatment was efficient in returning the AC adsorption capacity, maximum efficiencies of approximately 79% and 84% were reached when the Carbon Fiber Cloth-AC electrode was subjected to anodic and cathodic currents, respectively, at a current of 0.1 A. In addition, the material demonstrated good stability through adsorption-regeneration cycles by cathodic process, with the material's adsorption capacity being almost totally recovered for 8 consecutive cycles. The removal percentage around 80% was kept after the cycles, with optimal conditions when the electrode was subjected to cathodic currents, NaCl as electrolyte at a current of 0.1 A for 2 h. The characterization techniques provided results that allow to explain the higher and prolonged efficiency of the cathodic current. Furthermore, these reactor configurations achieved an electrical energy consumption of 2.3 and 2.1 kWh kg -1 of material for cathodic and anodic, respectively. These results indicate that the electrochemical is an economical and environmental suitable technique capable of restore carbon adsorbents to be reusable for several water treatment cycles.

- **Keywords:** Adsorption; Water treatment; Adsorbent recycling; Electrochemistry; Electrodesorption

Somu Mandal, Niroj Kumar Mohalik, Santosh Kumar Ray, Asfar Mobin Khan, Debashish Mishra, Jai Krishna Pandey. *A comparative kinetic study between TGA & DSC techniques using model-free and model-based analyses to assess spontaneous combustion propensity of Indian coals*. Pages 1113-1126.

Kinetic study of coal was carried out using simultaneous thermal analysis (STA) technique to assess the spontaneous combustion propensity of coal samples collected from various Indian coalfields having both fiery and non-fiery seams. The kinetic parameters were estimated by using both model-free and model-based analysis for both TGA & DSC data. The model-based method comprises four different consecutive reaction steps, viz. A→B→C→D→E for the spontaneous combustion process and the second reaction step (B→C) were used for this investigation. Chemometric analysis was applied to know the relation between the proximate analysis and activation energy of the samples using model-free and model-based techniques. The activation energy for the second reaction step of the model-based method for both TGA and DSC data showed a good relationship with the standard methods i.e., crossing point temperature (XPT) and Tgign of the samples. It indicates that the activation energy values at the oxidation stage (2nd stage) play a significant role in the spontaneous combustion propensity of coal. The study also reveals that the model-based analysis provided better results in comparison to model-free analysis to assess the spontaneous combustion propensity of coal.

- **Keywords:** Coal Spontaneous combustion; Kinetic Analysis; Model-free kinetics; Model-based Analysis; TGA-DSC

Jiyan Liu, Xinglong Liu, Jie Li, Junyao Ren, Jie Wang, Lanyi Sun. *Design and control of side-stream extractive distillation to separate acetic acid and cyclohexanone from wastewater by varying pressure*. Pages 1127-1149.

A large amount of wastewater containing acetic acid and cyclohexanone is produced during the production of ε-caprolactone. It is necessary to recycle acetic acid and cyclohexanone from wastewater. In this paper, the feasibility analysis for the separation of acetic acid/ cyclohexanone/ water with a near-azeotrope and an azeotrope which is pressure sensitive is carried out based on the residue curve map (RCM). And two sequences of conventional extractive distillation are determined. In order to prevent the remixing effect in conventional extractive distillation, four configurations of side-stream extractive distillation by varying pressure are proposed and optimized. The results show that the single liquid side-stream extractive distillation configuration SED1 is the optimal configuration in terms of economy, environmental protection, energy efficiency and safety. Compared with the optimal conventional extractive distillation configuration CED1, the total annual cost (TAC) of SED1 is reduced by 6.6%, and CO2 emissions are reduced by 11.9%. Subsequently, three proportion-integral (PI) control structures and a model predictive control (MPC) structure are proposed for SED1. The robustness and controllability of PI and MPC systems are compared by calculating integral absolute error (IAE). The findings indicate that the MPC structure has the best performance among all control structures.

- **Keywords:** Side-stream extractive distillation; Conceptual design; Inherent safety analysis; Distillation control; Model predictive control

Xuli Meng, Xuan Li, Long D. Nghiem, Eric Ruiz, Mohammed A. Johir, Li Gao, Qilin Wang. *Improved stormwater management through the combination of the conventional water sensitive urban design and stormwater pipeline network*. Pages 1164-1173.

With rapid urbanization, flooding events become more frequently in daily life, causing enormous economic damage and loss of life. Water Sensitive Urban Design (WSUD) is a common approach for mitigating stormwater runoff. However, it showed limited performance in big catchment areas (>1000 ha). This study proposed an innovative approach by combining conventional WSUD projects with the stormwater pipeline network through linear connections for better stormwater runoff management for a big catchment. The performance of combined WSUD projects and conventional WSUD was evaluated using the urban water system of a catchment (over 1200 ha) in Sydney, Australia, through the water mass balance modelling approach using annual rainfall data of 70 years (from 1950 to 2020). Combined WSUD reduced the stormwater runoff by over 124 ML/yr compared to that of the conventional WSUD model in accommodating future development. Combined WSUD restored the evapotranspiration and infiltration under high, average and low annual rainfall scenarios with an increasing 20–30% increase of evapotranspiration and infiltration in combined WSUD than the conventional WSUD. The results obtained from the study demonstrated that combining WSUDs with the stormwater pipeline network through linear connections is a promising approach in stormwater management and restoring the natural hydrological cycle.

- **Keywords:** Water Sensitive Urban Design (WSUD); Stormwater runoff; Hydrological cycle; Area-Pipeline-Policy (APP), stormwater management, stormwater pipeline network

Xiuwei Ma, Shouyuan Li, Yong Hou, Hao Lv, Jinjin Li, Tangying Cheng, Linjun Yang, Hao Wu. *Adsorption of low-concentration organic pollutants*

***from typical coal-fired power plants by activated carbon injection*. Pages 1174-1183.**

Activated carbon (AC) injection was applied to remove the organic pollutants from coal-fired power plants. The total hydrocarbon (THC) concentration in flue gases was 0.512–0.998 mg/m3, aromatic hydrocarbons and oxygenated volatile organic compounds (VOCs) were the major components. With the AC injection (150 mg/m3), the THC was removed by 36.52–46.49%. The mesopores could capture some larger organic molecules and facilitate the intrapore diffusion. Improving the AC injection amount promoted the organic pollutant adsorption, but lowered the AC adsorption capacity. Removal performance of organic pollutants was affected by their physicochemical properties. The removal efficiency for most VOCs was within the range of 15–50%, while that was 45–90% for semi-VOCs. Minor amounts of VOCs achieved high removal efficiency through specific interactions, especially oxygenated VOCs. However, the removal efficiency of the total oxygenated VOCs was lower due to competition adsorption with inorganic components. AC injection had no significant effect on the physicochemical properties of fly ash. This work and results provide a feasible method and reference for the reduction of organic pollutants in coal-fired power plants and other combustion exhaust gases.

- **Keywords:** Coal-fired power plant; Organic pollutants; Adsorption; Activated carbon injection; Fly ash

Fucheng Chang, Wei Li, Han Hu, Fanglan Ge, Guiying Chen, Yao Ren. *Chemical pretreatment and saccharification of corncob for poly-γ-glutamic acid production by Bacillus subtilis SCP010*-1. Pages 1184-1193.

Lignocellulosic biomass is an important raw material which has been extensively studied for biotechnological applications, but research on its use for the production of γ-polyglutamic acid (γ-PGA) is rarely reported. The present study aimed to improve the release of xylose and glucose from corncob for γ-PGA production using the strain Bacillus subtilis SCP010–1, which could metabolize xylose. The effectiveness of the three chemical reagents NaOH, NH3 and H2O2 pretreatments was investigated by the response surface methodology (RSM). The results showed that maximum glucose and xylose yields of 11.8 ± 0.3 and 17.36 ± 0.6 g/L, respectively, as determined by phloroglucinol-acid and enzymatic methods, were obtained when using 0.986% of NaOH for 2.07 h. Then, the pretreatment solution was subject to further optimize conditions of enzymatic hydrolysis, and the content of glucose and xylose in the corncob hydrolysate reached respectively 15.3 ± 0.3 and 22.34 ± 0.17 g/L under synergism of hemicellulase and cellulase. Finally, the fermentation conditions for γ-PGA production by B. subtilis SCP010–1 were also optimized, and after adding supplemental nutrients to the corncob hydrolysate, a maximum γ-PGA production of 30.035 ± 0.49 g/L was achieved by fed batch fermentation with feeding corncob hydrolysate. Considering the cost of the materials used in this study, nearly 85% of reduction in cost could be achieved, hence indicating that this production plan offers good prospects for industrial production of γ-PGA. More importantly, this process allows the use of environmental-friendly biological resources.

- **Keywords:** Lignocellulosic materials; γ-PGA; Corncob; Enzymatic hydrolysis; Saccharification

Eman G. Gamea, Ahmad Anwar, A.A. Ezzat, M. Essam El-Rafey. *Utilization of electric arc furnace dust as a filler for unsaturated polyester resin*. Pages 1194-1202.

Electric Arc Furnace Dust (EAFD) is a waste material produced during the steelmaking process. It contains a large amount of valuable metal oxides that can be used as a filling additive to improve the polymer properties. In this study, EAFD is used as a filler to the unsaturated polyester (UP) resin in different weight percentages. Neat UP and UP/EAFD compounds were studied mechanically by testing their tensile, impact, flexural, and hardness properties. The samples were investigated physically by density and water absorption, in addition to flammability analysis was performed by testing the Limiting Oxygen Index (LOI). Finally, the thermal properties were determined using Thermogravimetric Analysis (TGA). The result showed that the incorporation of the EAFD particles into the UP matrix has significantly affected the mechanical properties by increasing tensile strength up to 42%. The hardness of the UP/EAFD composites increases up to 8.5% and reaches a maximum value at 10 wt% of EAFD. Flexural strength and impact strength showed an optimal value at 5 wt% of EAFD. The flammability of the composites decreased by 34% at 30 wt% of EAFD. The thermal stability of the composites showed a remarkable increasing trend. Therefore, utilizing EAFD in UP matrix would help improve the environmental pollution control of the steel industry. Finding useful applications of this dust as a filler for the composite industry might convert this hazardous waste into a byproduct that should reduce the expenses and increase their profit.

- **Keywords:** Unsaturated polyester resin; Electric arc furnace dust; Thermoset; Industrial waste; Hazardous waste; Flame retardancy

Jiyun Wang, Mingyan Wang, Xiaoyang Yu, Ruowen Zong, Shouxiang Lu. *Experimental and numerical study of the fire behavior of a tank with oil leaking and burning*. Pages 1203-1214.

Leaking-burning coupling fires caused by oil leakage from tanks cause significant damage to occupants and the equipment. A series of experiments was conducted to investigate the fire behavior of a tank with oil leaking and burning. The tank released n-heptane into the tray below, forming a fire that heated the tank. The tray size and leak diameter varied. Spill fires, steady pool fires, boiling pool fires, and jet fires were observed. The results show that within a specific leak diameter range (2.5–3.5 mm), the maximum pressure increased with decreasing leak diameter. The fuel vapor spread along the bottom of the tank, causing the expansion of the flame. Consequently, the pool fire size was larger than the actual tray size, thereby making the maximum pressure and thermal radiation almost independent of tray size. When the leaking oil began to boil and burn, the pressure increased rapidly and the emitted radiative heat flux was the largest; therefore, fire posed the most serious threat. A computational fluid dynamics (CFD) modeling approach was employed to predict the time when the temperature of the leaking oil reached its boiling point. The predicted results were validated against the experimental ones, which provided useful support for emergency response plans.

- **Keywords:** Experiments; Oil tank; Leaking-burning; Thermal response; Thermal radiation; CFD modeling

Ahmed Elsayed, Ahmad Siam, Wael El-Dakhakhni. *Machine learning classification algorithms for inadequate wastewater treatment risk mitigation*. Pages 1224-1235.

Continuous monitoring of wastewater treatment processes is key to mitigate the risk of inadequately treated wastewater on the environment and public health. However, effective control of wastewater treatment processes is challenging because of the numerous relevant variables and their complex physio-chemical-biological interdependence. Most published related studies focused on correlating the effluent concentration of chemical oxygen demand and/or suspended solids using only a limited number of wastewater influent variables. In addition, recent machine learning- (ML)

based studies in wastewater treatment systems considered some individual classification algorithms rather than providing a comparison between different algorithm performances. In the current study, different algorithms were developed to categorize a range of wastewater treatment effluent characteristics based on multiple influent variables. To demonstrate their application, 23 ML classification algorithms were deployed on a wastewater treatment reactor-generated dataset and their performances were evaluated considering two different group of metrics related to the removal efficiency and effluent quality. The analysis results showed that, among all considered algorithms, the ensemble bagged trees algorithm had the most superior performance in terms of its overall classification accuracy. An interpretability analysis was further performed on the treatment process variables to detect the correlation between the input and output variables and to assess variable importance. In practice, the developed algorithms can facilitate optimal operation and effective management of wastewater treatment plants. ML algorithms also present efficient tools for rapidly classifying the effluent characteristics in lieu of typical sampling and laboratory analysis processes.

- **Keywords:** Machine learning algorithms; Wastewater treatment; Removal efficiency; Effluent quality; Bagging algorithms; Machine learning interpretability

Mao Yang, Li Yan, Yanchun Li, Pan Huang, Wenjia Han, Xugang Dang. *An environment-friendly leather waste-based liquid film mulching and its application for facilitating the growth of maize crops*. Pages 1236-1244.

Currently, environment-friendly high water-absorbing, water-retention, water-resistant, and water erosion resistance materials are the research hotspot in agricultural film. In this research, a new type of leather waste-based liquid film mulching (WG) was prepared by waterborne polyurethane (WPU) grafted with gelatin(G) extracted from leather waste. The interacting behavior of the prepared WG with soil particles was characterized including soil particles morphological changes, water-retention, water-resistant, water erosion resistance, and farming experiments. The SEM revealed that the WG could form a "coating layer" on the soil surface. The coating layer could improve the water-retention and water resistance of the soil. Meanwhile, the farming applications found that the soil sprayed WG could form a certain closed space which played a role in water-resistant, water erosion resistance, heat preservation, and moisture retention for maize. Especially, the water-absorbing, water-retention, and thermal-retention efficiency reached 80.5%, 20.2%, and 23.1 °C, respectively when the WG content was 50 g/m2 in the soil experimental sample. Moreover, after the WG was sprayed evenly on farmland, the germination period of the maize seeds was significantly shortened, the germination rate reached 92%, which was far higher than that of the bare soil. As an environment-friendly leather waste-based liquid film mulching, the WG could not only meet the growth of maize, increase yield, but also provide new ideas for the recycling of leather waste.

- **Keywords:** Leather waste; Gelatin; Waterborne polyurethane; Liquid film mulching; Agricultural production