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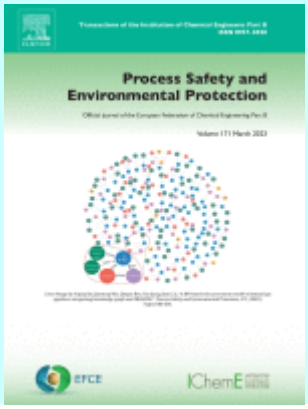

Dejun Miao, Yueying Lv, Kai Yu, Lu Liu, Jiachen Jiang. *Research on coal mine hidden danger analysis and risk early warning technology based on data mining in China*. Pages 1-17.

The development of intelligence and informatization is the inevitable trend of safety production in coal enterprises. Data mining technology plays an important role in promoting the development of coal mine safety management. This paper uses natural language processing technology and the Bi-LSTM model to automatically classify the hidden danger information and extract the theme of the coal mine. Then, taking the risk of a coal mine gas explosion as the starting point, the gas safety situation prediction model is constructed. Finally, an accurate management and control information system based on data mining technology and intelligent technology is developed, which realizes the information analysis of a large visual screen and the intelligent information processing of the APP. The system has been applied in the Luxi coal mine, and the application effect is good, which significantly improves the safety management ability and efficiency of the coal mine. This study can provide new ideas and methods for the dual pre-control construction of coal mines, strengthen the information processing capacity of the existing pre-control system, and promote the healthy development of the coal industry.

- **Keywords:** Data mining; Information system; Risk; Early warning; Safety; Coal mine gas explosion

Leila Samaddoost, Mahsa Soltani, Esmaeil Fatehifar, Ebrahim Abbasi Asl. *Design of amine-functionalized resin via a facial method with efficient CO2 capture from air*. Pages 18-27.

In this study, using A400 Purolite as a solid resin base, solid adsorbents were prepared for the direct adsorption of carbon dioxide gas from the ambient air. The resin was functionalized with different percentages of amine (TEPA). Then, the adsorption capacity was modified for better performance in the presence of STAB as a surfactant. Prepared samples were evaluated by CO2 adsorption and the experiments were done at identical conditions (22 °C, CO2 concentration 400 mg/L, and airflow of 2 L/min). The highest CO2

capture was related to sample with 40 % amines, whose adsorption capacity was 58 mg/g after 24 h. Then different amounts of the surfactants were added to these samples. Modified adsorbents in 10 % surfactants and 40 % amines (T40/S10 sample) showed the best performance by 84 mg/g CO2 adsorption in 24 h. The adsorption capacity of adsorbents increased after being functionalized with TEPA and the addition of STAB to the adsorbent surface, and led to increasing the adsorption capacity by 44 % (84 mg/g in 24 h). Also, the experimental results showed that the best performance of the adsorbent occurs at a loading of 0.5 gr and a gas flow of 0.3 L/min. Eventually, the influence of different operation parameters like adsorbent loading, airflow, and desorption temperature on the adsorbent performance in three cycles was investigated. Also, the reusability and stability of T40/S10 as the optimum sample was examined.

- **Keywords:** Solid Sorbent; CO2 Adsorption; Amine; Ion-exchange

SH. Khodaparast, V. Zare, F. Mohammadkhani. *Geothermal assisted hydrogen liquefaction systems integrated with liquid nitrogen precooling; Thermoeconomic comparison of Claude and reverse Brayton cycle for liquid nitrogen supply*. Pages 28-37.

Hydrogen liquefaction systems are of paramount importance in achieving a low liquid hydrogen price in developing the hydrogen supply chain. In these systems, reduction of compression work and efficient supply of liquid nitrogen for precooling purposes is essential. In this respect the present research proposes an investigation of two efficient configurations comprised of a Claude cycle for hydrogen liquefaction integrated with geothermal driven organic Rankine cycle to compensate some of the consumed power. In the proposed schemes, either the Claude or reverse Brayton cycles are employed and modeled for liquid nitrogen supply, while in most of previous research a fixed value was considered for compression work to supply the liquid nitrogen, reducing the accuracy of their reported outcomes. A comprehensive thermoeconomic assessment was implemented to determine a better scheme under various operating conditions using a parametric study. The results revealed the vital importance of integrated modeling of the liquid nitrogen supply unit with that of the hydrogen liquefaction system.

- **Keywords:** Geothermal; Hydrogen liquefaction; Reverse Brayton; Claude cycle; Exergoeconomic

Ankur Srivastava, Arunabh Meshram. *On trending technologies of aluminium dross recycling: A review*. Pages 38-54.

The objective of this review is to critically evaluate important aspects of aluminium dross generation, classification, properties, applications, and its commercial recycling techniques. A by-product of aluminium industry, aluminium dross is recycled by pyrometallurgy, hydrometallurgy, and hydrothermal processes, leading to aluminium recovery and generation of valuable products. The dominance of pyrometallurgy on the industrial scale is evident, owing to the efficient metal recovery processes, namely, Rotary salt furnace (RSF) and salt-free technologies (SFT). On the laboratory research front, hydrometallurgy and hydrothermal processes emerge as promising routes of dross recycling. Production of zeolites, ion exchangers, molecular sieves, and layered double hydroxides is achieved by hydrothermal route and important aluminium-rich products, along with gases like H2, CH4, and NH3 are produced by hydrometallurgical route. The advantages and disadvantages of each route govern the applicability of these processes. With a plethora of modern technologies emphasising on the recycling of aluminium dross, a detailed investigation of each route is vital. The recycling of dross also contributes to the judicious preservation of natural resources consumed during aluminium production. In addition, the adverse effects of improper dross disposal on human health and the environment have been discussed.

- **Keywords:** Aluminium dross; Recycling; Pyrometallurgy; Hydrometallurgy; Hydrothermal Processes

Oscar Kayanja, Mohsen A. Hassan, Ahmed Hassanin, Hidenori Ohashi, Ahmed S.G. Khalil. *Effect of phase disparity of MoS2 nanosheets on the performance of PES membranes for dual industrial oil-in-water emulsion separation and dyes adsorption*. Pages 55-70.

Water shortage is a global challenge due to increased demand and hence, reliable wastewater treatment avenues must be created to solve this problem. In this work, we report about the fabrication of dual performance polyethersulfone (PES) membranes modified with molybdenum disulfide (MoS2) nanosheets of different phases for wastewater remediation. We optimised process parameters to obtain large area, defect free membrane sheets. Comprehensive characterization revealed the phase disparity of MoS2, and changes introduced in the modified PES membranes. Blending MoS2 with PES membranes enhanced the mechanical properties as well as water uptake differently. The optimum PES membrane was modified with 0.2 wt% of 70% 1 T/2 H MoS2 and possessed superior pure water permeance of 778 kg/m2.h.bar. It also showed superior performance towards oil removal with rejection efficiency of 99% for 1 g/L oil concentration and it revealed excellent antifouling properties. The optimum membrane showed appreciable performance in organic dye rejection, even though it was outpaced by the 0.5 wt% of 70% 1 T/2 H MoS2 modified PES with a dye rejection of 98% towards methylene blue and 92% towards Rhodamine B. This work revealed that the phase of MoS2 strongly influences the structure and performance of the resultant PES-based nanocomposite membranes in ultrafiltration applications.

- **Keywords:** Nanocomposite PES membranes; 2D nanosheets; Oily wastewater separation; Cationic dyes separation

Haonan Ma, Weidong Zhang, Yao Wang, Yibo Ai, Wenyue Zheng. *Advances in corrosion growth modeling for oil and gas pipelines: A review*. Pages 71-86.

To quantify the progress of corrosion damage and develop pipeline integrity management strategies, it is necessary to establish a reliable corrosion growth model. Due to the complexity of the corrosion process, the availability of data, and the limitations of various models in their applicability, there is currently no generally accepted optimal corrosion growth prediction methodology. Corrosion data used for modeling, in-line inspection techniques for detecting defects, and sources of uncertainty in the modeling process are briefly described. This paper focuses on reviewing the concepts, the performance, and the application of existing pipeline corrosion growth models. The deterministic and probabilistic models are analyzed in detail according to the core methods involved, and the latest applications of machine learning and deep learning in corrosion growth modeling are also introduced. To leverage the strengths of various models, this paper presents hybrid approach models based on the combinations of the aforementioned models, which have greater performance and interpretability than single models and should be given more attention in the future development of corrosion growth prediction. Finally, some suggestions for future development are put forward in light of the challenges and deficiencies present in the current modeling process.

- **Keywords:** Corrosion; Probabilistic models; Machine learning; Hybrid approach models; Oil and gas pipeline; Corrosion rate

Maryam Dehbani, Hamed Rashidi. *Utilization of an innovative sono-microreactor for CO2 stripping from aqueous methyldiethanolamine solution*. Pages 87-97.

In the present study, a novel designed ultrasound-equipped microchannel reactor has been used to improve the CO2 desorption process from aqueous N-methyldiethanolamine (MDEA) solutions. CO2 desorption rate for a microreactor without ultrasound irradiation was compared with an ultrasound-equipped one at various temperatures, flow rates, and ultrasound powers. The results revealed that ultrasound vibrations could facilitate CO2 desorption and cause a significant increase in the rate of that through generation of cavitation bubbles and turbulence. Evaluation of energy and mass transfer characteristics was performed; 37.8% energy saving and 144.2% increase in mass transfer coefficient was obtained using ultrasound at its maximum power compared to microreactor without ultrasound irradiation. Also, comparisons between the designed sono-microreactor and conventional methods for CO2 desorption were performed in terms of desorption energy consumption and mass transfer coefficient, indicating 40.9% energy saving compared to 30 wt% MEA benchmark process and 160 times increase in mass transfer coefficient. Due to its high performance in terms of energy saving and mass transfer enhancement compared to the conventional method, the newly designed sono-microreactor can be introduced as a highly efficient technique for solvent regeneration.

- **Keywords:** CO2 desorption; MDEA; Ultrasound; Acoustic cavitation; Microchannel

Huan Liu, Dongxu Ji, Meng An, A.W. Kandeal, Amrit Kumar Thakur, Mohamed R. Elkadeem, Almoataz M. Algazzar, Gamal B. Abdelaziz, Swellam W. Sharshir. *Performance enhancement of solar desalination using evacuated tubes, ultrasonic atomizers, and cobalt oxide nanofluid integrated with cover cooling*. Pages 98-108.

The water shortage crisis has been paid attention to and many efforts have been conducted to find proper and applicable solutions to it through developing desalination systems. Commonly, being simple in construction and easy operation, solar stills (SSs) have been developed to meet the freshwater need; especially, in arid areas. However, their productivity and efficiency improvement are still a challenge. Accordingly, the current work aimed to enhance the thermo-economic performance of a pyramid SS (PSS) by augmenting the evaporation and condensation processes. For obtaining high vapor generation, evacuated tubes and ultrasonic foggers were integrated into the developed PSS (DPSS) as a first case (DPSS-I), in which different operation times of the foggers were tested. Then, Co3O4 nanofluid (1.5 wt%) was added as a basin fluid in the second case (DPSS-II). Finally, in the third case (DPSS-III), a glass cooling was used for boosting the condensation rate. Besides the experiments, a complete thermo-economic performance analysis was done via calculating the energetic and exergetic efficiencies and freshwater cost (per liter). All these performance indicators of DPSS were compared to that of traditional PSS (TPSS). As resulted, integrating all the proposed additives (DPSS-III) could enhance freshwater production, energy efficiency, and exergy efficiency by 83.87%, 18.29% and 38.86%, respectively. Additionally, the production cost, per freshwater liter, was reduced by 11.61%. These results showed the applicability, sustainability, and feasibility of the proposed additives in the field of solar desalination, particularly SSs.

- **Keywords:** Solar desalination; Evacuated tube; Ultrasonic foggers; Nanofluid; Energy efficiency; Exergy efficiency

Mabinty Sarah Tholley, Lartey Young George, Gehui Wang, Sajid Ullah, Zhihua Qiao, Siyuan Ling, Jinhong Wu, Cheng Peng, Wei Zhang. *Risk assessment and source apportionment of heavy metalloids from typical farmlands provinces in China*. Pages 109-118.

Potentially toxic metals in farmland soil have recently become a significant environmental concern in China. In this study, the occurrence and distribution of eight (8) heavy metals (HMs) were investigated from 54 topsoil samples obtained across 18 provinces. Human health and ecological hazards associated with HMs were assessed through different risk characterization indices and their sources predicted. The statistically mean concentrations of HMs ranged from 0.08 to 70.05 mg kg−1, which were below the determined threshold values for agricultural lands according to the Chinese National Standard (GB 15618–2018). The respective ecological risk index (Eri) of HMs revealed that they posed a lower risk (Eri<40) but their potential cumulative ecological risk (RI) was determined as a considerable risk (300 ≤ RI < 600). Spatial distribution and heterogeneities of HMs were found to be highly concentrated in the southern parts (e.g., Yunnan, Guangdong) of China, particularly for Arsenic (As), Zinc (Zn), and Chromium (Cr). PMF model was found capable of efficiently elucidating respective sources of HMs across the studied provinces as most were impacted by geological/pedogenic and anthropogenic activities (e.g., agricultural, industrial discharge fallouts). Probabilistic health risk assessment indicated that the non-carcinogenic risk (NCR) and total carcinogenic risk (TCR) of HMs in both adults and children were low and acceptable.

- **Keywords:** Farmland soils; Heavy metals; Multivariate analysis; Risk assessment; Source apportionment

Yuhuan Wang, Haiming Yu, Xianhang Yang, Sen Xie, Yuxi Ye, Chuangen Hou, Tianyuan Gao. *Study on the effect law of virtual impact separator efficiency based on multi-factor orthogonal test*. Pages 119-131.

In order to effectively solve the problem of low separation efficiency of respiratory dust in coal mine, a multi-factor orthogonal experiment was designed for the virtual impact separation device. A coupled airflow-dust migration model for describing the interior of the separator device was established based on the Euler-Lagrange method, and the 3D structure materializing of the separator was realized by accurate 3D printing technology. The maximum deviation of the separation efficiency between the experimental results and the simulation results is 5.85%. Through range analysis, the importance degree of each factor affecting the separation efficiency is determined as follows: nozzle diameter (20.31) > inlet section diameter (18.02) > distance between nozzle and large particle collecting cavity (14.85) > inlet length (10.66) > large particle collecting cavity diameter (10.04) > strong current sampling flow rate (7.84); The better separation scheme is found and the separation efficiency of dust with particle size of 1 μm~7 μm is 91.75%, 90.75%, 78.61%, 68.85%, 58.14%, 34.12%, 12.41%, respectively. The research results provide theoretical guidance for the development and application of virtual impact separation technology.

- **Keywords:** Dust monitoring; Respiratory dust; Virtual impact; Separation efficiency; Structural parameters

Li Gao, Xuan Li, Ming Li, Arash Zamyadi, Qilin Wang *Recent research advances in aqueous pollutants and treatment approaches*. Pages 132-135.

The water industry faces significant challenges under the impacts of climate change, population growth, and water resource scarcity. Great efforts and progress have been made to understand the presence and behaviors of emerging contaminants, their health

and environmental impacts, and the energy-efficient and cost-effective treatment technologies. In this 'Aqueous Emerging Pollutants and Treatment' special issue, we collect 32 articles to demonstrate recent research progress in aqueous pollutants and treatment approaches. An overview of these 32 articles is provided. Six main trends for future research in aqueous pollutants and their treatment technologies have been provided.

Nagehan Şahin, Rahim Şibil. *Hydrodynamic performance evaluation of screening on the physical unit operations in wastewater treatment based on experimentally validated CFD computations*. Pages 136-151.

This paper introduces an evaluation of the hydrodynamic performance of the flow in the screens used on the physical unit operations in a selected full-scale wastewater treatment plant (WWTP) based on Computational Fluid Dynamics (CFD) simulations. The numerical study was carried out with the ANSYS Fluent, CFD software by using the three-dimensional (3 D), steady, incompressible flow based on the Reynolds-Average Navier-Stokes equations with three different turbulence modeling. The hydrodynamic behavior of the screening facility, combined with head pond-upstream channel-bar screens was evaluated under different conditions of the mass flow rate and velocity fields. Also, the numerical study was validated against the experimental study, which implemented in-situ measurements by Acoustic Doppler Velocimeter (ADV), and consistent results were obtained between the numerical and experimental study. Interestingly, while the Realizable (real) k-ε turbulence model with the relative error of 9.31% gave the best predicting results in the head pond, the renormalization group (RNG) k-ε turbulence model with the relative error of 9.05% gave the best predicting results in the upstream channel and through bar screens. As a result of the experimental measurements and CFD analyses carried out in the full-scale WWTP, the function of the screening facility was found to be incomplete. Moreover, a hydraulically improved new geometry was presented to operate the existing WWTP efficiently.

- **Keywords:** CFD modeling; Screening; Turbulence modeling; Acoustic Doppler Velocimeter

Mohammad Tahmasebzadehbaie, Hoseyn Sayyaadi. *Techno-economic-reliability assessment of a combined NGL refinery and CCHP system driven by wasted energy of flare and flue gases*. Pages 152-166.

Due to their improved functionality and increased efficiency, hybrid flare and flue gas recovery methods have drawn attention. Applying these methods removes flare gas in the oil wells and hot flue gas in the power plant, and a combination of flare gas recovery with hot flue gas recovery is more environmentally friendly as it increases the energy efficiency of the technologies. Integrated heating, cooling, and electricity generation plants composed of a gas turbine, a natural gas liquids refinery, and an absorption chiller were proposed as a hybrid system for flare and flue gas recovery in an oil well. The generated cooling was used in the natural gas liquids refinery and inlet air cooling of the gas turbine. Thermo-economic analysis was applied to the system with consideration of the recovery of heat from the gas turbines' hot flue gas. The reliability of its downstream installation was examined. The sensitivity analysis showed that the proposed system is very economical even at low electricity prices, and the most sensitive equipment is the NGL's recovery section.

- **Keywords:** Flare and flue gas recovery; Reliability; Markov technique; Water-ammonia absorption chiller; CCHP

Zhanwei He, Xiaojun Hu, Kuo-Chih Chou. *Oxidative modification of industrial basic oxygen furnace slag for recover iron-containing phase: Study on phase transformation and mineral structure evolution*. Pages 167-175.

Basic oxygen furnace (BOF) slag is the main co-product in the steelmaking process, its recycling within the iron and steel enterprises is crucial for the industry to ensure greater sustainability. According to the composition characteristics of BOF slag, a method of separating and recovering iron resources by regulating the composition of BOF slag with silica as an additive at high temperature was proposed. In this study, the growth of iron-containing phase during oxidative modification of BOF slag was in-situ observed by ultra-high-temperature confocal scanning laser microscope, and the phase transformation and mineral structure evolution were analyzed by chemical analysis, X-ray diffraction and field emission scanning electron microscopy. The results demonstrated that the increase of oxidation temperature effectively promoted the transformation of iron oxides to (Mg,Fe2+)O·Fe2O3, but too high temperature could lead to the increase of iron-containing melilite phase and reduce the iron recovery. In the oxidative modification process, the appropriate holding time and cooling mode facilitated the growth and development of (Mg,Fe2+)O·Fe2O3 particles, which was conducive to the separation and recovery of iron resources. After BOF slag was oxidized at 1300 ℃ for 240 min and cooled in the furnace (1 ℃/min), the grade of magnetic slag obtained by magnetic separation had a grade of 40.26%, a recovery of 70.95%, and a P and S content of 0.042 and 0.456, respectively, which may be used as an important supplement to the raw materials for sintering. The regulated secondary slag may be used to diversify into higher value-added production. Therefore, the systematic research and development of oxidative modification-crushing-magnetic separation technology may promote the efficient utilization of BOF slag components and heat energy.

- **Keywords:** Industrial BOF slag; Modification; Phase transformation; Structure evolution; Magnetic separation

Siwen Li, Hongbin Yu, Yingzi Lin, Suiyi Zhu, Gen Liu, Chunyan Shi. *Sulfamethazine degradation by sulfite through GAC@Ni/Fe Three-Dimensional (3D) particle electrode activation: Contribution of active substance and synergy*. Pages 176-187.

The widespread production and use of antibiotics, which accumulate in the environment and lead to chronic poisoning of non-target organisms, causing potential safety risks to the environment and human health. In this study, GAC@Ni/Fe was used as particle electrode and sulfite hetero activator for synergistic degradation of Sulfamethazine(SMR) in a three-dimensional electrode reactor. Under the optimal experimental parameters (trough voltage = 5 V, sulfite addition =1 mM, particle electrode addition = 40 g, PH = 7), the removal rate of SMR can reach 96.91% within 30 min. The surface changes before and after the reaction at the GAC@Ni/Fe particle electrode was characterized using XRD, XPS, and FTIR. LSV, Tafel, and EIS were used to investigate the electrochemical performance of the GAC@Ni/Fe particle electrodes. The superiority of Three-Dimensional(3D) (GAC@Ni/Fe)/Sulfite system in SMR removal was confirmed by comparative experiments and reaction synergistic factor analysis. Electron paramagnetic resonance (EPR) and quenching experimental studies demonstrate that the degradation of SMR within the 3D (GAC@Ni/Fe)/Sulfite system is the result of both free radical and non-free radicals, with·OH, SO4−·and 1O2 contributing 51%, 12% and 37% to SMR removal, respectively. The 54.57% TOC removal rate (30 min) also demonstrates the efficient mineralization of SMR by the system. The results show that the 3D (GAC@Ni / Fe) / Sulfite system can be used to treat the wastewater containing SMR and other antibiotics, which is a green and ecologically friendly method with potential application value.

- **Keywords:** GAC@Ni/Fe particle electrode; Sulfite; Electrocatalytic oxidation; Synergistic degradation; Reaction mechanism

Yun Zhong, Jie Shi, Kexin Li, Huiqin Guo, Liushui Yan, Zhenxing Zeng. *Silicotungstic acid as electron transfer mediator in Z-scheme g-C3N4/H4SiW12O40/Ag3PO4: Accelerated charge interface transportation for high-efficient photocatalysis*. Pages 188-199.

Photocatalytic degradation of organic pollutants has shown its promise in wastewater purification, however the photocatalytic activity on most catalysts are still unsatisfactory due to the poor reactive oxygen species production as a result of sluggish charge separation. Here, an innovative silicotungstic acid mediated charge transfer system over the Z-scheme g-C3N4/H4SiW12O40/Ag3PO4 photocatalyst is proposed, exhibiting remarkable photocatalytic activity toward oxygen activation for reactive oxygen species generation. We verify that the H4SiW12O40 with the unique Keggin units could serve as charge transfer mediator to speed up charge transportation between g-C3N4 and Ag3PO4, as a result showing dramatically enhanced charge separation efficiency. By virtue of the aforementioned advantages, the as-prepared Z-scheme photocatalyst of g-C3N4/H4SiW12O40/Ag3PO4 shows excellent photocatalytic performance toward carbamazepine degradation, where the pseudo-first-order rate constant is estimated to be 78, 18, and 9 times higher than that of g-C3N4, Ag3PO4, and g-C3N4/Ag3PO4. The innovative design of using H4SiW12O40 as solid charge transfer mediator offers new viewpoints in designing high-efficient photoctalysts for environmental related applications.

- **Keywords:** Z-scheme photocatalysis; Carbon nitride; AgNO3; Silicotungstic acid mediated charge transfer; Organic pollutants degradation

Haifeng Gong, Xin Luo, Yang Yang, Chen Huo, Ye Peng, Bao Yu, Haohua Zhang. *Structural optimization and separation characteristic of a separating device for three phases: Oil, water and solid*. Pages 200-213.

Solid particles and water are widely used as lubricating oils. However, oil–water–solid separation is inefficient when conventional methods are used. Therefore, a device is proposed to simultaneously separate oil, water, and solids from one another. In this study, a numerical model was established by combining the mixture, Reynolds stress, population balance, and discrete-phase models to investigate the separation characteristics of a separating device. The effect of the structural parameters on the separation was investigated, and the important structural parameters were optimized using the response surface method. The results indicate that the optimal underflow pipe, certain pipe, and sideflow pipe diameters are 6.5, 13.49, and 7 mm, respectively; at this instant, the tangential velocity in the small cone section and certain structure is large, the oil volume fraction is low near the underflow pipe, and the number of solid particles separating from the sideflow outlet increases, and the deoiling rate and desolidification rate reach a maximum of 84.45% and 91.44%. This study can provide valuable guidance for the design of high-performance devices for lubricating oil purification using physical methods.

- **Keywords:** Oil–water–solid phase separation; Lubricating oil; Separation efficiency; Structural optimization; Response surface methodology

Xujia Tang, Weipeng Lu, Xuefeng Yan. *Dual attention bidirectional generative adversarial network for dynamic uncertainty process monitoring and diagnosis*. Pages 214-224.

In industrial process monitoring, uncertainty in a system arises when measured data are not representative of actual data. Uncertain information should be extracted to maintain safe manufacturing. Interval value methods are generally used to monitor uncertainty in systems, and these methods assume the same uncertainty among variables. However, the variables of the same process differ in uncertainty. Moreover, the dynamic nature of the system causes a more complex uncertainty. To monitor and diagnose such processes, a fault-sensitive bidirectional generative adversarial network (FSBiGAN) is proposed. First, to extract valuable characteristics from uncertain input, BiGANs with self-attentive mechanisms are put in place. Second, a sensitive variable selection approach is utilized to create new fault-sensitive indicators capable of adapting to the dynamic changes of each process. Third, the variable selection approach is applied once more to identify variables causing a fault to occur. Finally, the self-attentive and sensitive variable-picking algorithms can be combined with other generative models to identify defects and analyze the dynamic properties of the process. Comparative experiments applying traditional monitoring and interval methods on the Tennessee Eastman dataset injected with differential uncertainty validate the effectiveness of FSBiGAN in monitoring and diagnosing dynamic uncertainty systems.

- **Keywords:** Uncertainty Process; Generative Adversarial Network; Self-Attentive Mechanism; Fault Detection; Fault Identification

Mengchu Wei, Aifang Pan, Runyong Ma, Hui Wang. *Distribution characteristics, source analysis and health risk assessment of heavy metals in farmland soil in Shiquan County, Shaanxi Province*. Pages 225-237.

Soil heavy metal pollution can cause irreversible harm to the ecological environment and human health. A total of 678 surface soil samples and 60 crop samples were collected to study the contamination level, source of heavy metals and human health risk in agricultural soil in central Shiquan County. The results show that the arithmetic mean values of chromium, copper, zinc, arsenic, lead, nickel, cadmium, and mercury in the soils of the study area were 1.67, 2.17, 1.73, 1.25, 1.24, 1.86, 5.04 and 2.17 times of their background values, respectively. However, the risk control standards for agricultural soil pollution in China were not exceeded. The high-value areas of soil heavy metals Cr, Cu, Zn, Ni, Cd, and Hg are mainly distributed in the northwest-southwest area of the study region. The results of the geo-accumulation index (Igeo) showed that the pollution levels of heavy metals in soil were in the order of Cd (0.98) > Cu (0.40) > Hg (0.20) > Ni (0.19) > Zn (0.14) > Cr (0.06) > Pb (−0.30) > As (−0.81). In addition, the soil cadmium contamination factor (CF) was 5.04, the pollution load index (PLI) was 2.97, which were significantly higher than other metals contamination levels. It indicates that cadmium pollution reaches a high level. Correlation analysis and principal component analysis (PCA) showed that Cr, Cu, Zn, As, Ni, Cd and Hg in soil were mainly derived from industrial pollution, while Pb was derived from soil parent material. The soil environment in the study area will not cause non-carcinogenic effects on adults and children. It is necessary to pay attention to the high risk of cancer caused by Cr in local residents. The excessive rate of heavy metals in vegetable crops in the study area was significantly higher than that in paddy. The results can provide basic information for soil heavy metal control and crop planting planning in Shiquan County.

- **Keywords:** Heavy metal; Soil; Source identification; Health risk assessment; Crops

Ziyang Li, Weijun Tian, Meile Chu, Mengyuan Zou, Jing Zhao. *Molecular imprinting functionalization of magnetic biochar to adsorb sulfamethoxazole: Mechanism, regeneration and targeted adsorption*. Pages 238-249.

Sulfamethoxazole (SMX), a typical medical antibiotic, is regarded as a major risk in the surface hydrosphere because of its harmful biological reaction and potential to trigger bacterial resistance. Ameliorating the hydrosphere will become more convenient if the challenging adsorption and separation of SMX in hydrosphere are achieved. To reveal the mechanism, regeneration and targeted adsorption of SMX on a novel surface-imprinted polymer (MIP-MBC) and batch experiments were carried out in this study. MIP-MBC was prepared in organic solution using a Fe-Mn-modified biochar to selectively adsorb SMX in a water solution. Owing to the mesopores and oxygen-containing functional groups of MIP-MBC, imprinted cavities in pores are found to lead to a remarkable adsorption efficiency for SMX. The maximum adsorption capacity for SMX reaches up to 25.65 mg g−1, which is 1.34 times that of the non-molecularly imprinted magnetic biochar (NIP-MBC). The adsorption process matches well with the second-order kinetics and Freundlich thermodynamic model, which indicates that hydrogen bonds and electrostatic interactions are simultaneously involved in the adsorption process. After five cycles, the adsorption rate for MIP-MBC reaches 88.34%. Furthermore, MIP-MBC is applied to the binary system to remove SMX, and it can be used to accurately identify and adsorb SMX due to K` > 1 and being independent of the ion concentration. The high affinity site plays a major role in the imprinting process for SMX. This study furnishes a novel perspective for promoting the practical application and economic benefits of targeted biochar material to capture SMX in sewage purification.

- **Keywords:** Sulfamethoxazole; Molecularly imprinted; Biochar; Adsorption

Jia Wang, Li Liu, Li'ao Wang, Jianhua Lu, Yujie Li. *Volatile methyl siloxane separation from biogas using hollow fiber membrane contactor with polyethylene glycol dimethyl ether: A numerical and experimental study*. Pages 250-259.

In this study, a mass transfer model for hollow fiber membrane contactors (HFMC) was developed to theoretically investigate the mass transfer performance of volatile methyl siloxane (VMS) separation by HFMC. In addition, the effects of operating parameters such as filling rate, liquid and gas velocities on the effectiveness of HFMC separation of VMS were experimentally investigated. The experimental results showed that the increase of filler fraction improved the removal of siloxane. When the absorbent velocity was 250 mL/min and the gas velocity was 500 mL/min, the removal rates of L2, D4, and D5 were 74%, 92%, and 89%, respectively. Additionally, the fluxes of L2, D4 and D5 also increased with the increase of gas and liquid velocities, which were in good agreement with the calculated results of the mass transfer model. The faster the gas and liquid velocities, the higher the total mass transfer coefficient, which indicated that the mass transfer resistance was reduced in the contactor system. The liquid phase mass transfer resistance contributed the most to the total mass transfer resistance in the non-wetting model. However, when the membrane was 10% wetted, the mass transfer resistance contribution of the membrane increased sharply, reaching a maximum of 38.2%.

- **Keywords:** Biogas; Volatile methyl siloxane; Hollow fiber membrane contactor; Model development

Xinhong Li, Jingwen Wang. *Modelling underwater dispersion of gas released from seabed soil considering current and wave*. Pages 260-271.

Subsea gas release incidents may result in catastrophic consequences, e.g., overturning of offshore floating structures, fire, and explosion. This paper developed a model to investigate the dispersion behavior of underwater gas released from the seafloor soil under combined action of current and wave. Eulerian-Eulerian model is used to track underwater gas dispersion trajectory. Porous model is utilized to describe the seafloor soil and simulate the penetration of gas released from seafloor soil. The numerical model is validated by comparing with small-scale experiments. The effect of release rate, current velocity and soil porosity is investigated. The parameters, e.g., rising time, horizontal dispersion distance and surfacing area are estimated. The uniqueness of this study is that underwater gas plumes are simulated considering the seafloor soil and the combined action of current and wave. The results indicate that the presence of seafloor soil has a significant effect on the migration shape and trajectory of underwater gas plume. The combined action of current and wave increases the dispersion distance of gas plume. This study can support risk assessment and emergency planning of subsea gas release accidents.

- **Keywords:** Underwater gas release; Current and wave; Numerical model; Seafloor soil

Anita Nagarajan, Bernard Goyette, Vijaya Raghavan, Adarsh Bhaskar, Rajinikanth Rajagopal. *Nutrient recovery via struvite production from livestock manure-digestate streams: Towards closed loop bio-economy*. Pages 273-288.

Phosphorous and Nitrogen are key nutrients for plants growth, usually supplemented by in the form of fertilizers. Therefore, management and utilization of these compounds in a sustainable manner for agriculture is of importance to serve the rising global demand of food. One way is to valorize agricultural wastes in many different ways like anaerobic digestion, struvite production and so on to maximize nutrient recovery and reduce wastage. Struvite recovery is one of the green marketing tools in the fertilizer industry, given the high amount of agriculture and livestock wastes produced. While struvite can be produced from a wide range of wastewater, this article provides an overview about struvite with an emphasis about its production from anaerobic digestates, manure and livestock wastewater and its prospective as a source of fertilizer. Furthermore, discussions about integration with anaerobic digestion, cost benefits and post application plant yields are reviewed to show its practicality and commercial potential. Despite constraints, struvite production promotes circular bioeconomic, sustainable process with a high nutrient recovery and this review will aid to take decisions in implementing this method in the near future.

- **Keywords:** Nutrient Recovery; Circular Bioeconomy; Struvite; Anaerobic Digestion; Waste Management; Fertilizer

Jose Delgado, Wenel Naudy Vásquez Salcedo, Christine Devouge-Boyer, Jean-Pierre Hebert, Julien Legros, Bruno Renou, Christoph Held, Henrik Grenman, Sébastien Leveneur. *Reaction enthalpies for the hydrogenation of alkyl levulinates and levulinic acid on Ru/C– influence of experimental conditions and alkyl chain length*. Pages 289-298.

The development of process flow diagrams requires knowledge of reaction enthalpy for pinch analysis and thermal risk assessment. Such information is missing for some biomass processes, such as the production of γ-valerolactone (GVL) from the hydrogenation of levulinic acid or alkyl levulinate. To fill this gap, this manuscript

describes a detailed calorimetric study on the hydrogenation of levulinic acid (LA), methyl levulinate (ML), ethyl levulinate (EL), propyl levulinate (PrL), butyl levulinate (BL) and pentyl levulinate (PeL) over Ru/C. This reaction system occurs through a two-step pathway with a domino hydrogenation/cyclization sequence. The cyclization step (lactonization) was found to be endothermic and was evaluated by a Tian-Calvet C80 micro-calorimeter, whereas the hydrogenation step was found to be exothermic and was tracked by a RC1 Mettler Toledo High-Pressure calorimeter. It was verified that reaction enthalpy is independent of reaction temperature (in the operating conditions used in this work), levulinate concentration and solvent (levulinate, corresponding alcohol or GVL). It was also found that reaction enthalpy for both steps did not depend linearly on alkyl chain length.

- **Keywords:** Tian-Calvet calorimeter; RC1; Hydrogenation; Levulinate; Levulinic acid

Yuan Xu, Xue Jiang, Wei Ke, Qunxiong Zhu, Yanlin He, Yang Zhang, Zixu Wang. *A novel pattern classification integrated GLPP with improved AROMF for fault diagnosis*. Pages 299-311.

With the scale expansion of industrial processes, safety has become one of its important links and the requirements for safety monitoring are getting higher. How to realize timely and effective fault diagnosis, especially for incipient faults, has attracted more discussion and research. This paper proposes a novel pattern classification integrated global−local preserving projections (GLPP) and improved adaptive rank-order morphological filter (IAROMF) for fault diagnosis. First, in order to preserve the global manifold information and local manifold information of the data, GLPP is introduced to extract the features of the data to obtain the test signal and the template signal. Second, AROMF transformation is performed on the test signal and template signal to obtain the output trend feature. Third, as the pattern matching by Euclidean distance-based AROMF has the restriction of sequence timing and the feature points need to be strictly corresponding, the Weighted Dynamic Time Warping (WDTW) distance is used to calculate the total error of iteration between the template trend and the output trend. In order to prove the effectiveness of the method proposed in this paper, a case study was carried out on the Tennessee Eastman (TE) process. The experiment results illustrated that the novel pattern classification method proposed in this paper has higher diagnostic accuracy than other fault diagnosis methods, especially for incipient faults.

- **Keywords:** GLPP; AROMF; WDTW distance; Pattern classification; Fault diagnosis

Tao Hai, Yujun Bai, Wurood Yassen, Ali E. Anqi, Ahmed Deifalla, Shunsuke Nakamura, Wejdan Deebani, Meshal Shutaywi. *Development of a novel geothermal trigeneration system utilizing modified organic-flash cycle and zeotropic mixtures: Environmental assessment and optimization*. Pages 312-329.

Due to the rise in global energy demand caused by growth in the human population and standards of living, renewable energy-based trigeneration systems have gained importance recently. Owing to this, an innovative geothermal-powered trigeneration system is presented to produce electricity, H2, and cooling simultaneously. Also, its performance is scrutinized from the thermodynamic, environmental, and sustainability outlooks to find the best zeotropic mixtures. A two-objective optimization is conducted, taking into account both energetic and exergetic efficiencies as objectives to detect the optimized working conditions. The used mixtures include Butane/Pentane, Butene/Pentane, Isobutene/Pentane, Isobutane/Pentane, R142b/Pentane, R236ea/Pentane, and R245fa/Pentane. Based on studies of the mass fraction of Pentane, the Isobutene/Pentane mixture exhibits the best performance among the zeotropic

mixtures. For the Isobutene/Pentane mixture, a rising flash tank temperature leads to reduced net electricity and produced H2 rate, whereas the cooling load goes up. Furthermore, the energetic efficiency of the system has an increasing trend with increments in the temperature of the evaporators in the design. With increasing temperature of the evaporators and flash tank temperature, the CO2 emissions rate has an increasing trend. Finally, there is a considerable amount of exergy destroyed by the vapor generator in both optimal and base operating conditions.

- **Keywords:** Bi-evaporator systems; Environmental assessment; Optimization; Sustainability; Zeotropic mixtures

Hang Zhang, Shuo Chen, Liyu Ran, Hongtao Yu. *Enhanced PMS activation by surface electronic reconstruction at Co3O4/ZnO heterointerface: Performance and mechanism*. Pages 330-340.

Peroxymonosulfate (PMS) activation is regarded as a powerful method for eliminating refractory organic pollutants. A PMS catalyst with a rapid electron-transfer capability is vital for the generation of active species. Herein, an efficient Co3O4/ZnO catalyst with abundant Co3O4-ZnO heterointerface is synthesized by calcining Zn3[Co(CN6)]2 prussian blue analogues. Such a heterointerface can induce electron redistribution due to different work function between Co3O4 and ZnO, as confirmed by XPS characterization. Owing to the electron redistribution at Co3O4-ZnO heterointerface, a faster electron-transfer between catalyst and PMS is achieved, as proved by electrochemical studies. A series of controlled experiments, characterization and density functional theory calculation suggest that the fast electron transfer benefits from the enhanced electron-donating ability of Co(II) and the increased active sites (oxygen vacancy). Therefore, Co3O4/ZnO-3 shows superior catalytic activity toward PMS than Co3O4. The pseudo-first-order kinetic constant for phenol degradation by Co3O4/ZnO-3 (0.31 min−1) is 4 times higher than that of Co3O4. Besides, other refractory organic pollutants including bisphenol A, sulfamethoxazole, ibuprofenand and rhodamine B could also be degraded effectively by Co3O4/ZnO-3 system. This study highlights how the interface design can optimize the electronic structure for enhanced catalytic activity and provides a new strategy to develop efficient PMS catalyst.

- **Keywords:** Heterogeneous catalysts; Composite metal oxides; Heterointerface; Electron redistribution; PMS activation

Hailin Yu, Huili Zhang, Xin Wei, Yong Chen, Bo Yu, Yingjun Wang, Hongsheng Liu. *Preparation of a cationic block copolymer composite coagulant TP(AM-DAC-PPFS) and its coagulation performance for treating oilfield sewage.* Pages 341-352.

Efficient purification of oily sewage, recycling, and standard discharge have become key issues for the sustainable development of oil fields. In this study, the surface of PPFS was organically modified by a silane coupling agent. Then, covalently bonded cationic block inorganic-organic composite coagulant was prepared by chosen sodium polyacrylate as the template. This unique structure significantly enhances the positive charge and molecular chain length of the coagulant, thus improving its ability to perform charge neutralisation, adsorption bridging, and sweep coagulation. The characteristic functional groups and thermophysical properties of the composite coagulant were analysed by FTIR and thermogravimetric analysis. The transformation of random copolymers to block copolymers was determined by 1 H NMR, thus confirming the successful synthesis of the cationic block structures. The turbidity removal and oil removal properties of oily sewage were investigated by coagulation experiment. The Zeta potential, dynamic and static light scattering, and field emission scanning electron microscopy (SEM) were used to study the effect of composite coagulants on the microscopic morphology and coagulation of flocs.

Finally, the coagulation mechanism of the compound coagulant was analyzed with the dynamic change of the particle size of the flocs. The cationic block structure in TP(AM-DAC-PPFS) can effectively neutralise the negative charges on the surface of impurity particles and emulsified oil. The optimal dosage of TP(AM-DAC-PPFS) was 30 mg·L−1, at which the turbidity and oil removal rates can reach 98.3% and 93.8%, respectively.

- **Keywords:** Compound coagulant; Cationic microblock; Oily sewage; Coagulation mechanism; Floc morphology

Yi Wu, Haotian Ye, Hong-guang Dong. *An inherently safer design approach based on process safety time for batch chemical reaction processes*. Pages 353-364.

The economic attractiveness of an industrial process depends a large extent on its safe and reliable operation. The inherently safer design can help reduce the potential hazard on a fundamental level and eliminate escalation at the early stage of process development. In this work, an inherently safer design method for batch chemical reactors is proposed, which maximizes the yield of target product while minimizes Dow's fire and explosion index. Process safety time is introduced as criterion to respond to the thermal runaway risk risen by unexpected failures. Finally, two examples for specific reaction systems with given kinetics are performed to demonstrate the feasibility and validity of the proposed method. The results indicate that the product yield optimized with the proposed method is significantly higher than that obtained from literature approach involving temperature limit or divergence criterion under the same PST. With the same yield, the PST optimized with the proposed method is longer.

- **Keywords:** Multi-objective optimization; Inherent safer; Process safety time; Batch reactor; Thermal runaway criterion

Hanlin Wang, Ziming Xu, Can Cheng, Teng Wang, Meng Mei, Si Chen, Jingxin Liu, Jinping Li. *Unveiling effect of iron on pyrolysis of bisphenol A epoxy by comparisons of product characteristics and reaction mechanisms*. Pages 365-373.

Bisphenol A epoxy (BAEP) is a widely-used material in daily life, and increasing BAEP wastes are being generated. Pyrolysis is a potential technology for BAEP recovery, but conventional processes are inefficient and high energy-consuming. Herein, Fe-catalyzed pyrolysis process was proposed, and comprehensive comparisons were performed on characteristics of products obtained from BAEP pyrolysis in the presence and absence of iron. The results demonstrated that the addition of iron reduced the decomposition temperature of BAEP by approximately 10–20 °C and promoted the generation of gaseous products, in addition, the appropriate conditions were determined as the iron content of 4%, pyrolysis temperature of 400 °C, holding time of 90 min, and heating rate of 5 °C/min. Moreover, based on the analyses of Py-GCMS for volatiles and XPS for residues, the catalytic mechanism was revealed as the facilitation effect of iron on the conversion of lattice oxygen to adsorbed oxygen. This work would be conducive to energy saving and light products production during BAEP pyrolysis and offer valuable references for studies on the recovery of some other organic materials/wastes.

- **Keywords:** Bisphenol A epoxy; Catalytic pyrolysis; Product yields; Iron conversion; Oxygen vacancy

Muhammad Kamran, Ridho Kresna Wattimena, Danial Jahed Armaghani, Panagiotis G. Asteris, Izhar Mithal Jiskani, Edy Tonnizam Mohamad. *Intelligent based decision-making strategy to predict fire intensity in subsurface engineering environments*. Pages 374-384.

The prospect of subsurface structures taking uncontrollable fire is a significant cause of stress held by people from all over the world. Mine fires and explosions have caused countless casualties and material losses for decades. A fire in a mine has the ability to rapidly contaminate the air of the entire mine, which might result in the loss of life and, in certain cases, the suspension of mining industry processes. Mine fires deplete coal supplies, release greenhouse gases and toxic chemicals, and cause ground subsidence from coal volume loss. This study aims to explore some interesting aspects of mine's fire data using Catboost and light gradient boosting machine (LightGBM) methods in order to minimize the human fatalities and material losses during the construction of deep underground engineering projects. Firstly, 120 samples demonstrating several distinct characteristics were gathered from an underground coal mine in Turkey. The prediction framework was developed employing the training set and the appropriate configuration of hyperparameters. The findings indicate that LightGBM algorithms achieved a more comprehensive performance in comparison with Catboost, with an accuracy of 92 % and 89 %, respectively. Hence, the proposed intelligent decision-making model can be employed in preventing and warning system of fire risks in subsurface engineering projects. The suggested strategy would serve as a reliable guide for predicting fire intensity in deep underground projects to ensure safe subsurface environments. This research promotes safe, hygienic, environmentally friendly, climate-smart and sustainable development by reducing greenhouse gas emissions.

- **Keywords:** Fire; Environment; Safety; Sustainable growth; Subsurface Structures; Green Mining

Huixing Meng, Qiaoqiao Yang, Enrico Zio, Jinduo Xing. *An integrated methodology for dynamic risk prediction of thermal runaway in lithium-ion batteries*. Pages 385-395.

The risk of thermal runaway in lithium-ion battery (LIB) attracts significant attention from domains of society, industry, and academia. However, the thermal runaway prediction in the framework of system safety requires further efforts. In this paper, we propose a methodology for dynamic risk prediction by integrating fault tree (FT), dynamic Bayesian network (DBN) and support vector regression (SVR). FT graphically describes the logic of mechanism of thermal runaway. DBN allows considering multiple states and uncertain inference for providing quantitative results of the risk evolution. SVR is subsequently utilized for predicting the risk from the DBN estimation. The proposed methodology can be applied for risk early warning of LIB thermal runaway.

- **Keywords:** Lithium-ion battery; Thermal runaway; Risk prediction; Dynamic Bayesian network; Support vector regression

Xiaobing Gao, Qiusheng Zhou, Yilin Wang, Tiangui Qi, Leiting Shen, Guihua Liu, Zhihong Peng, Xiaobin Li. *Coal fly ash resource utilization: Structure of siloxy group of high-modulus sodium silicate solution*. Pages 396-404.

To achieve the deep separation and resource utilization of alumina and silica in aluminosilicate solid wastes such as coal fly ash and coal gangue, the siloxy group structures of high-modulus sodium silicate solution under various moduli (1.5 – 3.0), sodium oxide concentrations (30 – 70 g·L−1) and thermal histories were studied as well as the solution properties of pH and viscosity. The results show that the polymerization

degree of silicate anions and the solution viscosity increase with increasing modulus, and the solution structure becomes complex with a predominance of high-polymeric sheet (Q3), chain (Q2) and cage-like (Q4) groups, whereas the pH of the solution decreases. Although the number of high-polymeric siloxy groups increases with increasing temperature, neither increasing the temperature nor prolonging the residence time is conducive to the polymerization of high-polymeric siloxy groups. The polymerization degree and the number of silicate species increase with increasing sodium oxide concentration for solutions with a constant modulus. The viscosity of high-modulus solutions increases conspicuously due to the presence of siloxy groups with the higher polymerization degree, but the increase in pH is not significant.

- **Keywords:** Sodium silicate solution; Polymerization degree; Siloxy group; Silicate species

Peng Xu, Zhuoyu Yang, Xin Liu, Pengfei Zhu. *Synergistic enhancement of ferrous ion with zero-valent copper/oxygen system: In-site formation and catalysis of H2O2*. Pages 405-412.

Zero-valent copper (ZVC) coupled with oxygen gas (O2) was extensively studied to degrade refractory contaminant, while the active dismutation reaction and low reactivity of Cu(I) refrained the performance at acid condition. In this study, ferrous ion (Fe(II)) was added to the ZVC/O2 system (ZVC/Fe(II)/O2 system) to enhance the degradation ability, the degradation rate of acid orange 7 in the ZVC/Fe(II)/O2 system was enhanced by 34.8% compared to the ZVC/O2 system, and the corresponding apparent rate constant was almost three times higher than that of the ZVC/O2 system. In the reactive species identification experiments, by electron spin resonance experiments and quenching experiments of nitrobenzene, tert butyl alcohol and methanol, hydroxyl radical was proven as primary reactive oxygen species rather than high-valent metal-Cu(III). In addition, the optimum ZVC dosage, Fe(II) concentration, pH and stirring rate were derived based on optimization experiments combined with economic applicability. In the ZVC/Fe(II)/O2 system, the mechanism was analyzed by detecting the variation of the concentration of H2O2, Cu(I) and total dissolved copper in the solution. In the degradation process, ZVC was corroded to form Cu(I) by H+, then Cu(I) reacted with O2 to generate hydrogen peroxide, the generated hydrogen peroxide was induced by Fe(II) and Cu(I) to produce hydroxyl radical, at the same time, ZVC and Cu(I) could reduce Fe(III) to Fe(II). The coexisting substances like carbonate ion, nitrate ion, sulfate ion and phosphate ion did not affect the demineralization of acid orange 7 in the ZVC/Fe(II)/O2 system, chloride ion remarkably accelerated the degradation rate of acid orange 7, while fulvic acid limited the acid orange 7 removal. The ZVC/Fe(II)/O2 system also showed excellent degradability in well water, lake water and tap water. Total dissolved copper concentration was controlled within 1 mg/L by the alkali precipitation method, which was within II-level environmental quality criteria in China. These facts suggested that Fe(II)-enhanced ZVC system had great development potential in water treatment.

- **Keywords:** ZVC/Fe(II)/O2 system; •OH; Circulation of Fe(III)/Fe(II); In-site generation of H2O2; Acid orange 7 degradation

A. Sangeetha, R. Gandhimathi, P.V. Nidheesh. *Treatment of stabilized landfill leachate using pyrite-activated persulfate oxidation process*. Pages 413-422.

Landfill leachate is a major hazard for the surrounding ambience as it detrimentally contaminates the soil and groundwater. In the present study, sulfate radical based advanced oxidation process (SR-AOP) was adopted for the treatment of stabilized/mature landfill leachate (SLL) using pyrite (FeS2) as a heterogeneous catalyst. The FeS2 catalyst was characterized using XRD, FT-IR, SEM and EDX spectroscopy techniques to evaluate its structural, functional groups, morphological features, and chemical composition,

respectively. The effect of various operating parameters on SR-AOP such as initial pH, FeS2 dosage, Na2S2O8 concentration, and temperature on COD and TOC removal was also studied. The FeS2 (1000 mg/L), Na2S2O8 (1000 mg/L) concentrations at pH 8.8 were found optimal, and COD and TOC removals were found as 78.5% and 74.2%, respectively. After the treatment of SR-AOP, BOD5,20/COD ratio of landfill leachate was improved from 0.023 to 0.41. Scavenging tests revealed that the primary oxidative species in SR-AOP are •OH and SO4•-; however, SO4•- plays a major role while •OH is also involved in the process. Intriguingly, no significant change in the catalytic efficiency and characteristic nature of FeS2 was observed even after four sequential treatments of the same FeS2 catalyst.

- **Keywords:** Landfill leachate; Advanced oxidation process; Sulfate radical; Pyrite; Heterogeneous catalyst

Junying Song, Chunhui Zhao, Xiao-qiang Cao, Weimin Cheng. *Enhanced catalytic degradation of antibiotics by peanut shell-derived biochar-Co3O4 activated peroxymonosulfate: An experimental and mechanistic study*. Pages 423-436.

A peanut shell-derived biochar-Co3O4 (Bio-Co3O4) catalyst prepared by chemical bath deposition (CBD) method exhibited excellent ofloxacin (OFL) degradation ability through a broad pH range for peroxymonosulfate (PMS) activation. The excellent properties and behavior of catalyst were studied by characterization and degradation experiments. Benefiting from the synergy of adsorption and degradation, Bio-Co3O4 composite showed much higher removal efficiency (97.3%) and larger reaction rate constant ($k = 0.1411\ min^{-1}$) than that of biochar or Co3O4 in presence of PMS. Mechanisms exploration suggested that dual active pathways, including singlet oxygen-dominated non-radical pathway and sulfate radical-dominated radical pathway were involved in the reaction mechanism. The graphitized structure, stable redox cycle of Co2+/Co3+ and CO groups in catalyst were mainly responsible for the generation of reactive species. Furthermore, a total of ten main intermediates were detected and OFL degradation pathways as well as catalytic mechanisms were identified and proposed in detail. Overall, our study provides a potential way to activate PMS for the effective removal of abusive antibiotics from aqueous environments.

- **Keywords:** Peroxymonosulfate; Ofloxacin; Singlet oxygen; Composite catalyst; Mechanism

Meng Zhang, Xiong Cao, Baolin Li, Aitao Zhou. *Quantitative study on the role of desorption gas on coal-gas outbursts: Energy contribution and dynamic characteristics*. Pages 437-446.

Coal-gas outburst is a violent phenomenon of energy release and strong dynamics is generated in underground coal mining. Coal-gas outbursts are accompanied by strong coal pulverization, and the gas desorbed by pulverized coal will in turn promote the development and spread of outbursts. Quantitative study on the role desorption gas played can improve the disaster-causing mechanism of coal-gas outburst and guide the work of outburst prevention and disaster reduction. Based on established gas emission model, the gas desorption is combined with the outburst process and its dynamic characteristics in this paper. The energy contribution and outburst dynamics with desorption gas are quantitatively studied under various desorption conditions, verified by outburst experiments. The results indicate that the energy contribution of desorption gas is 15.49–58.59% for JG71 coal, 4.49–57.26% for JG82 coal. The coal pulverization in the JG82 coal seam has a great influence on the energy contribution of desorption gas. After correction of gas desorption, the energy contribution increases by ~20%. The maximum energy release rate (MERR) of the outburst with 0.075–0.15 mm JG71 coal sample

reaches is 2.87 times that of the 1–2.36 mm coal sample at 3 MPa, and even 5.72 times that of the JG82 coal sample. For the outburst experiments, the energy contribution of desorption gas is 31.97–40.06% with 1–2.36 mm coal, 50.29–52.76% with < 0.25 mm coal. This paper presents a novel quantitative study defining the role of gas desorption in outburst energy and dynamics, applicable to disaster risk assessment and an accurate method to derive the energy contribution of desorption gas in experiments is proposed.

- **Keywords:** Coal-gas outburst; Gas emission model; Desorption gas; Energy contribution; Dynamic characteristic

Xiaoxiang Wang, Tong Wei, Yuce Wen, Chunya Yang, Dong Ye, Sujing Li, Wei Li. *Catalytic ozonation of toluene and dichloromethane mixture at low temperatures over modified MnOx-based catalyst*. Pages 447-458.

Catalytic ozonation is an efficient method for VOCs abatement at low temperatures, in which the rational design of highly active heterogeneous catalysts constitutes the most significant step. In this study, Al2O3 was first optimized by loading MnOx. And then K was used for modifying MnOx/Al2O3 catalyst, which exhibited 2.4 × 10−3 mol·g−1·s−1 oxidation rate for dichloromethane and toluene oxidation with ca. 0.89 ppm ozone detected at 80 °C. That could be directly applied for removing toluene and dichloromethane mixture or coupled with other treatment technologies (such as biological purification). Besides, appropriate K doping could increase the amount of reactive surface oxygen species and the ratio of Mn2+, hence contributing to an enhanced oxidation ability. By contrast, an excess K doping inevitably lowered the activity of active surface oxygen species and interfered with the transformation of Mn3+ to Mn2+, which resulted in a weakened oxidative ability and thus a decreased catalytic activity. Finally, the reaction mechanisms over 0.1 K-MnOx/Al2O3 were tried to be demonstrated that the degradation of toluene mainly followed the pathway of toluene – phenylcarbinol – benzaldehyde – benzoic acid – phenyl group – small-molecule species and/or CO2 while the route of dichloromethane – methanol – formaldehyde – formic acid – small-molecule species and/or CO2 explained the catalytic oxidation of dichloromethane. All of these findings may facilitate the design of novel heterogeneous catalysts for VOCs oxidation and progress the development of catalytic ozonation for toluene and dichloromethane abatement.

- **Keywords:** Catalytic ozonation; Toluene and dichloromethane; MnOx-based catalyst; K modification; Redox ability

Cao Fang, Changsheng Shao, Shenhao Wang, Yahui Wu, Chao Liu, Qing Huang. *Simultaneous removal of levofloxacin and sulfadiazine in water by dielectric barrier discharge (DBD) plasma: Enhanced performance and degradation mechanism*. Pages 459-469.

Antibiotics are abused and discharged into environmental water, posing a constant potential threat to ecosystem. It is still a challenge to treat the wastewater containing various antibiotics. While many studies have reported the plasma treatment of different antibiotics, how to treat multiple antibiotics simultaneously with high efficiency still remains an unsolved problem. In this work, we employed atmospheric-pressure dielectric barrier discharge (DBD) to treat levofloxacin and sulfadiazine as two typical antibiotics in water, and investigated the treatment efficiency and the involved mechanism. The experimental results indicated that under proper conditions, the total antibiotics removal efficiency could be enhanced compared to separate single antibiotic treatment. The contributions from the plasma-induced reactive oxygen/nitrogen species (RONS) were examined, showing that ·OH played a major role in levofloxacin degradation, while ozone and peroxynitrite also played a certain role in sulfadiazine degradation. The bio-toxicity evaluation for the plasma treatment of levofloxacin and sulfadiazine was also provided,

showing that the DBD degradation products were harmless to the ecological environment. As such, this work may not only provide a practical solution to treatment of wastewater containing multiple antibiotics, but also give the insights into the mechanism for the efficient DBD treatment of mixed antibiotics in wastewater.

- **Keywords:** Antibiotics; Dielectric barrier discharge (DBD); Levofloxacin; Sulfadiazine; Degradation; Bio-toxicity

Challa Mallikarjuna, Rajesh Roshan Dash. *Statistical analysis of treatment of rice mill wastewater using the aerobic inverse fluidized bed biofilm reactor (AIFBBR)*. Pages 470-481.

Among the different industries, the ricemill industry is identified as one of the major polluting industries because of the large amounts of effluents generated and variations in the concentration of its constituents. The current experimental study aimed to investigate the treatment of ricemill (simulated) using the aerobic inverse fluidized bed biofilm reactor (AIFBBR). Box–Behnken design (BBD) based statiscal response surface methodology (RSM) was used for the current AIFBBR-ricemill treatment system. For the evaluation of the RSM process through the BBD technique, three input variables: Influent COD (800–3200 mg/L), HRT (12–24 h), and % bed volume (15 – 45), and two output variables: %COD and %TOC removal, were selected. The effect of these chosen variables was verified by conducting 15 experiments in a multivariate system for the AIFBBR-ricemill treatment system. The quadratic polynomial models yielded a regression coefficient (R2) of 0.99 (for both COD and TOC) when the experimental data were fitted to it, which indicates the model's suitability for the process. The precision and efficiency of the model were visualized using the ANOVA and lack of fit test. The system has witnessed the maximum COD (88.95%) and TOC (95.68%) removal at optimum parameters of 2804.27 mg/L of influent COD, 23.79 h of HRT, and at a % bed volume of 44.94. Along with the COD and TOC, parameters such as nutrients (NH4+-N, PO43--P, and NO3--N), phenol, and lignin were also monitored in the present study.

- **Keywords:** Ricemill wastewater; AIFBBR; BBD; ANOVA; COD; TOC; Phenol; Lignin

Qiangling Duan, Huiqi Cao, Xiaoxi Li, Jinhua Sun. *Effects of urea on the thermal decomposition behavior of ammonium nitrate: A reliable thermal safety performance enhancer*. Pages 482-492.

To address the actual disaster of thermal decomposition and explosion of ammonium nitrate (AN), a commonly used raw material, urea was selected as an additive to study its effect on the thermal decomposition of AN through experimental and theoretical methods. The thermal decomposition kinetics, energy release, self-reaction properties of adiabatic environments, and escaping gaseous products have all been discussed. It was found that urea has an inhibitory effect on the crystalline transformation of AN stored at room temperature, which is beneficial to its thermal safety. The results showed that urea increased the activation energy of the thermal decomposition of AN, raised the temperature of the initial reaction and reduced heat generation. Furthermore, the action mechanism of urea is suggested to be heat absorption by its thermal decomposition and the escape of ammonia. Finally, the study carried out an engineering assessment of the thermal safety of AN under the action of urea and found that the addition of urea greatly enhanced the thermal safety performance of stored and transported AN. The comprehensive analysis concluded that a small dose of urea could be added to enhance the thermal stability of AN without affecting its normal function.

- **Keywords:** Ammonium nitrate; Urea; Thermal decomposition; Thermal hazards; Safety prediction

Jianjun Hou, Shuxun Li, Lingxia Yang, Xuedong Zhang, Qian Zhao. Multi-leakage source localization of safety valve based on improved KDE algorithm. Pages 493-506.

The safety valve is the core component of the safety pressure relief protection device of the pressure-bearing special equipment. When the safety valve leaks, the medium of the pressure vessel will be lost and wasted, which may lead to safety accidents. Aiming at the problem that it is difficult to accurately locate multiple tiny leak holes in safety valves, multi-leakage source localization of safety valve combining the acoustic emission (AE) test with improved approximate kernel density estimation (KDE) algorithm is proposed. The algorithm first introduces the improved wavelet threshold function denoising method to extract the time-frequency support domain which is less affected by environmental noise and the energy of the leaked sound source is dominant, which makes the premise of the application of the KDE algorithm established. In the aspect of improving the wavelet threshold function, an improved adaptive wavelet threshold noise reduction method is proposed by using the decay characteristics of the exponential function. On this basis, the high-frequency aliasing is suppressed by frequency division fusion processing, the approximate kernel density function is calculated, and the three-dimensional spectral base of the approximate kernel density function is reduced. Through numerical calculation, the location coordinates of the leakage source of the safety valve are obtained according to the peak value of the improved KDE spectrum. The results show that the relative errors of the leakage location results of safety valves with working pressures of 0.72 MPa, 0.75 MPa and 0.77 MPa are all within 10%. The method of combining the acoustic emission test with the improved KDE algorithm can accurately locate the leakage source of the safety valve, and with the increase of the working pressure of the safety valve, the positioning accuracy is also improved accordingly.

- **Keywords:** Safety valve; Leak source location; Acoustic emission signal; Wavelet noise reduction; Frequency division processing

Maghsoud Abdollahi Haghghi, Zahra Mohammadi, Mostafa Delpisheh, Ebrahim Nadimi, Hassan Athari. *Multi-variable study/optimization of a novel geothermal-driven poly-generation system: Application of a soft-computing intelligent procedure and MOGWO*. Pages 507-531.

Due to the operational conditions of flash-binary geothermal cycles, it is difficult to design a multiple heat recovery technique for its waste heat. To address this deficiency and reuse its waste heat in different stages, this study proposes a novel poly-generation model considering parallel and series waste heat recovery. The prime target is to maintain the temperature and enthalpy level of the waste heat from each stage to another and provide a unified framework, leading to producing the main required products. The model comprises a transcritical carbon dioxide Rankine cycle, a desalination subsystem, a single-effect absorption refrigerator, and a low-temperature electrolyzer. To this end, a multi-aspect feasibility study is conducted from energy, exergy, and economic viewpoints, and a multi-criteria optimization is applied in four different scenarios using an artificial neural network in tandem with a multi-objective grey wolf optimization. The most suitable state of operation of each optimized scenario and the efficient scenario is defined through the TOPSIS approach. It was found that the most influential parameter affecting the performance metric was the geothermal water inlet temperature. Besides, the second scenario, i.e., exergy efficiency/total investment cost rate, resulted in the best state of operation. Finally, the optimum objective functions were gauged at 29.59% and 72.72 $/h, respectively. In this situation, the optimum net output power, cooling load, freshwater production rate, and hydrogen production rate were equal to 1666.0 kW, 1029.0 kW, 146.4 m3/day, and 1967.0 m3/day, respectively. Besides, the sustainability index and levelized cost of products were obtained to be 2.11 and 0.0602 $/kWh.

- **Keywords:** Poly-generation model; Geothermal cycle; Transcritical carbon dioxide Rankine cycle; Waste heat recovery; Artificial neural network; Grey wolf optimization

Uthradevi Kannan, Shihabudheen M. Maliyekkal. *A resource-efficient and portable nanotechnology-enabled disinfection system: Performance studies and a novel strategy to recycle spent material*. Pages 532-540.

The paper describes developing a point-of-use disinfection system consisting of a film-forming nanocomposite packed in a nylon sachet. The composite film consists of silver nanoparticles embedded in a matrix containing chitosan, reduced graphene oxide, and tannic acid. The long-term ability of the portable sachet bag to release silver ions and disinfect surface and groundwater is demonstrated. The sachet bag's disinfection potential is demonstrated by taking Escherichia coli MTCC 443 as the model microorganism. The system produced a complete and consistent 3 log10 reduction of E. coli over multiple cycles of use. The paper also describes a green recycling approach to utilise spent composite film and prevent AgNPs from entering the waste stream. The spent nanocomposite film is transformed into a concrete micro-crack sealant through a soft chemical route. The sealant's ability to plug micro-cracks in concrete is demonstrated, and the mechanism of sealant interaction with concrete is proposed. The sealant can fill cracks and solidify in an alkaline environment. The concrete cube specimens repaired with sealant showed enhanced compressive strength compared to the residual concrete cube specimens. The possible leaching of residual silver from the sealant in concrete is investigated via toxicity characteristic leaching procedure analysis. The study demonstrates that silver leaching is negligible (< 0.05 mg/L) and well below the permissible limit of 5 mg/L.

- **Keywords:** Water treatment; Portable disinfection unit; Silver-nanocomposite; Micro-crack sealant; Waste recycling; Waste-to-wealth

Yuan-Pin Shia, Bor-Yih Yu. *Development of a rigorous and generalized model on the hydrothermal liquefaction (HTL) process for bio-oil production*. Pages 541-554.

A rigorous process model for hydrothermal liquefaction (HTL) of microalgae is proposed in this work. This research attempts to uncover a complicated simulation scenario for the characterization of microalgae, the development of suitable reaction pathways, kinetics, and thermodynamics. In this study, 55 model compounds and 41 individual reactions were used to describe an HTL system. The kinetic parameters were regressed using literature data, which reported the results under different operating conditions using the three species of microalgae. The proposed kinetic model revealed acceptable predictivity by predicting 117 published biocrude yields (total 160) to within ± 10 wt% and 28 published HHV (total 39) to within ± 5 MJ/kg. Finally, a continuous HTL process was conceptually designed. The trade-off between the biocrude yield and HHV was investigated via multi-objective optimization (MOO), which yielded the best trade-off between the biocrude yields (37.2–60.0 wt%) and HHV (27.5 and 33.5 MJ/kg). This work presents a satisfactory first attempt to rigorously simulate a very complex HTL process. Its application in the preliminary process design, optimization, and economic analysis is recommended.

- **Keywords:** Hydrothermal liquefaction (HTL); Microalgae; Bio-oil; Process design; Simulated annealing; Multi-objective optimization

Zhan Li, Pengfei Zhang, Kecheng Guan, Ralph Rolly Gonzales, Toru Ishigami, Ming Xue, Tomohisa Yoshioka, Hideto Matsuyama. *An experimental study on recovering and concentrating ammonia by sweep gas membrane distillation*. Pages 555-560.

Ammonia is a toxic and hazardous substance, as well as a valuable chemical. The gaseous ammonia are soluble in water, rendering some industrial wastewater contains high concentration of ammonia. These wastewater can be a direct source for the production of commercially concentrated ammonia solution via sweep gas membrane distillation (SGMD). Taking advantage of vapor-liquid equilibrium of ammonia-water binary system, ammonia can be recovered from these wastewater, and concentrated to several times higher concentration under optimized conditions. In this work, we have demonstrated the ammonia recovery by SGMD process, and comprehensively investigated the effect of different operation conditions on the SGMD performance.

- **Keywords:** Ammonia recovery; Sweep gas membrane distillation; Vapor-liquid equilibrium; PVDF membrane; Operation condition optimization

Ahmed I. EL-Seesy, Mahmoud S. Waly, Hesham M. El-Batsh, Radwan M. El-Zoheiry. *Enhancement of the diesel fuel characteristics by using nitrogen-doped multi-walled carbon nanotube additives*. Pages 561-577.

Nanoparticles are considered promising additives to diesel fuel and significantly affect engine performance and exhaust emission levels. Nitrogen-doped multiwalled carbon nanotubes (N-doped MWCNTs) are one of the effective catalysts owing to their promising properties, which have recently increased their usability in many applications. These features make them good candidates as a catalyst to enhance diesel engine performance. The effects of adding N-doped MWCNTs into diesel fuel for a single-cylinder CI engine working at a rated speed of 1500 rpm and different loads were studied. Four doses of N-doped MWCNTs were added to diesel fuel using ultrasonic dispersion. Multiwalled carbon nanotubes (MWCNTs) were used as reference additives to compare their results with those obtained by N-doped MWCNTs. The results illustrated that most blends of N-doped MWCNTs were preferred in combustion behavior, engine performance, and exhaust emission analysis with respect to diesel and MWCNTs blends. Thus, there was a significant increase in the in-cylinder pressure and heat release rate compared to pure diesel. Also, the brake thermal efficiency was increased, and the brake specific fuel consumption was reduced compared to diesel. For all N-doped MWCNTs blends, there were remarkable reductions in NOx, soot, and CO formations, and it is mainly preferred over MWCNTs/diesel blends in exhaust emissions reduction.

- **Keywords:** Nitrogen-doped multiwalled carbon nanotubes; Diesel engine; Multiwalled carbon nanotubes; Combustion characteristics; Exhaust emission

Zhanguo Su, Yiping Su, Hasan Sh. Majdi, Ali Shawabkeh, Syed Zaheer Abbas, Sayed M. Eldin, Ahmed Deif, Hadi Ghaebi. *4E analyses of a novel multi-generation system based on methanol-steam reforming integrated with scramjet multi cooling cycle and ammonia synthesis*. Pages 578-590.

A state-of-art multi-generation plant integrated with a scramjet multi-cooling cycle for power, hydrogen, ammonia, and freshwater generation was analyzed from an energy, exergy, exergoeconomic as well as environmental (4E) standpoint. The coolant of the cooling cycle was the fuel of the scramjet cycle and in terms of optimizing consumed power, this cycle is benefiting from four-stage compressors. To improve the rate of hydrogen production, a methanol steam reforming procedure was employed. To provide fresh water, a reverse osmosis membrane was employed and integrated into the plant.

To consider the powers of input design variables on the implementation criteria of the plant and reduce CO and CO2 emission, an exhaustive parametric investigation was performed. The thermodynamic efficiencies, the sum unit cost of the products, the system emission rate, and the environment penalty cost rate as well as values of the products as the multi-generation plant's performance criteria were computed. Raising the hydrogen mole fraction caused an increase in the emission rate.

- **Keywords:** Methanol-steam reforming; Environmental analysis; Scramjet cycle; Thermoeconomic analysis; Ammonia synthesis

S. Karthick Raja Namasivayam, Subramanian Srinivasan, Krishnappa Samrat, Bala Priyalakshmi, Ramkumar Dinesh Kumar, Arvind Bharani, Ramkumar Ganesh Kumar, M. Kavisri, Meivelu Moovendhan. *Sustainable approach to manage the vulnerable rodents using eco-friendly green rodenticides formulation through nanotechnology principles:a review*. Pages 591-606.

This review provides an insight into the nanotechnology principles for plant-based rodenticides formulation and how they can be developed and superior to the conventional rodent control program. Development of Phyto or green nano rodenticides involves the selection of plant material, extraction of rodenticidal metabolites, formulation of plant extracts as Nanoparticles (Polymeric, Nanocapsules, Nanospheres, Solid, Lipid), Nanoemulsion, Nanocomposite, Nanoliposomes via green science or green technology principles, characterisation of nanoformulation like morphology, surface topology, functional group determination using electron microscopy, spectroscopy and X-ray crystallography. The effectiveness of the nanosystem can be proved by the determination of loading, entrapment efficacy and release profile. Bioassays studies with the respective nanoformulation under laboratory and field trials tests reveal Nanorodenticides. The stability of the respective nanoparticulate formulation can be assessed by zeta potential measurement. After the successful validation, it is necessary to study biocompatibility or biosafety using a suitable in vitro and in vivo screening model system that can be assessed through cell lines and zebrafish models. Any sign of toxic effect that can be measured in the respective model system reveals outstanding biocompatibility. This review demonstrates that the Nano Phyto rodenticides formulated by green nanotechnology can be potentially used to control rodents in an eco-friendly manner with high efficacy.

- **Keywords:** Rodents; Nano rodenticides; Metabolites; Nanoformulation; Nanomaterials; Biocompatibility

Yuanyuan Chen, Qingrui Zhang, Kang Liu, Siyuan Zhang, Xuehui Zhang, Hong Liu. *Simulation, optimization and intensification of the process for co-production of ethyl acetate and amyl acetate by reactive distillation*. Pages 607-618.

A new energy-saving process is proposed here for the co-production of ethyl acetate (EtAC) and amyl acetate (AmAC) by reactive distillation(RD). The thermodynamic feasibility of the ethyl acetate/amyl acetate system was determined based on its physical properties. As amyl acetate has a higher water-carrying capacity than ethyl acetate, water can be removed from the reaction system in the form of azeotrope to improve the conversion rate, and amyl acetate can be easily separated from the water. The reactive distillation process of ethyl acetate-amal acetate co-production with different alcohol feed ratios was studied in this paper. When the amyl alcohol to ethanol feed mole ratio was set at 2, the process performed better in terms of economy and energy consumption; it also had a less environmental impact at the same time. The reactive distillation process with intermediate condenser and intermediate reboiler (RD-IC-IR) process and the

reactive dividing-wall column (RDWC) process are established based on process optimization. Compared with the RD process, the TAC and CO2 emissions for the RD-IC-IR process reduced by 21.92 % and 28.27 %, respectively, and the thermodynamic efficiency improved 38.86 %; the TAC and CO2 emissions for the RDWC process reduced by 36.11 % and 42.49 %, respectively, and the thermodynamic efficiency improved 74.45 %.

- **Keywords:** Co-production of ethyl acetate-amyl acetate; Reactive distillation; Reactive distillation process with intermediate condenser and intermediate reboiler; Reactive dividing-wall column; Process optimization; Process evaluation

Yongjun Li, Zhirong Wang, Xuemeng Shi, Rujia Fan. *Safety analysis of hydrogen leakage accident with a mobile hydrogen refueling station*. Pages 619-629.

The operation of mobile hydrogen refueling stations will be popular for hydrogen energy supply in the future, and the investigation includes the hydrogen diffusion behavior of hydrogen leakage and the potential risk of explosion is pivotal to commercializing the mobile hydrogen refueling station. The dispersion of hydrogen leakage and the minimum safe distance of explosion of the mobile hydrogen refueling station are studied by simulation. The 3D full-scale geometry is established. Experimental data verifies the numerical models. The effects of the ventilation scenarios of the truck container and the ambient wind (wind speeds and wind directions) on hydrogen volume and diffusion distance are analyzed. By calculating the severe working conditions results, the hydrogen volume in the open space and the hydrogen concentration in the four 3-way corners of the ceiling in the truck container are obtained. Finally, the overpressure caused by hydrogen explosion is evaluated, and the minimum safe distance under different damage effects is predicted. The obtained results reveal that the conditions included that the side door and side window are open, low ambient wind speed, and wind direction from front to rear of the mobile hydrogen refueling station increase the risk of hydrogen leakage and diffusion. Based on severe working conditions, the average hydrogen volume is 87.9 m3 in the air in stable status. In the case of a hydrogen explosion, the minimum safe distance is 313.2 m. The investigation provided a valuable reference for evaluating and preventing hydrogen leakage accidents of the mobile hydrogen refueling station.

- **Keywords:** Hydrogen leakage; Hydrogen volume; Diffusion distance; Minimum safe distance; Mobile hydrogen refueling station

Alaa Mohamed, Samy Yousef, Simona Tuckute, Andrius Tonkonogovas, Arūnas Stankevičius. *Gas permeation and selectivity of polysulfone/carbon non-woven fabric membranes with sponge and finger-like structures*. Pages 630-639.

This research aims to investigate the effect of supporting polysulfone (PSF) membranes with different pore structures (sponge "SP" and finger "FP") by non-woven carbon fibers (CF) on their gas permeability and selectivity for different gas mixtures (H2/CO2, H2/N2, and H2/CH4) to avoid the lower mechanical strength of the commercial membranes. The thickness of the PSF layer was modified during the preparation process using a phase inversion approach. The impact of the support CF fabric and different pore structures on the mechanical, chemical, thermal, permeability, and selectivity characteristics of the fabricated membranes were examined. The results revealed a strong incorporation between PSF and the fabric, resulting in enhanced pores, increased porosity and higher roughness. The FP membrane's structure was found to have a smaller pore size of 56 nm, higher porosity (73.6%), surface roughness (44 nm) and higher strength (15.7 MPa) but less thermal stability (−36%) compared to the SP structure. Moreover, the SP structure exhibited higher gas permeability, particularly for H2, with

improvements of 32% for H2 and CO2, 25% for CH4, and 10% for N2. Furthermore, the PSF/CF membrane with SP structure exhibited higher selectively with 15.8%, 26.9%, and 14.4% improvements for H2/CO2, H2/N2, H2/CH4, respectively, compared to FP membranes. These results suggest that CF fabric has great potential as a membrane substrate and PSF/CF membranes with SP structures have high potential for use in the H2 gas separation process in harsh environments.

- **Keywords:** Polysulfone; Carbon fiber nonwoven fabric; Sponge-like structure; Finger-like structure; Hydrogen separation

Yiping Bai, Jiansong Wu, Qingru Ren, Yao Jiang, Jitao Cai. *A BN-based risk assessment model of natural gas pipelines integrating knowledge graph and DEMATEL*. Pages 640-654.

As one of the most essential process facilities, the natural gas pipeline may be affected by various hazards and result in frequent accidents. Although Bayesian Network (BN) and other methods have been applied for risk assessment of gas pipelines, most attempts rely on experts instead of data. In this paper, a novel risk assessment model integrating Knowledge Graph (KG), Decision-Making Trial and Evaluation Laboratory (DEMATEL), and BN is proposed to analyze gas pipeline accidents in a data-driven way to minimize the reliance on experts for the current BN-based approach. First, the KG is used to extract and illustrate the causal network from accident reports on the Internet instead of a limited number of experts. Then, DEMATEL is applied to quantify the complex correlations in the causal network to simplify the topology structure and convert it into a BN structure. Moreover, by conducting BN analysis, a probabilistic causation model of gas pipeline accidents is established to identify critical hazards, predict potential consequences and optimize risk reduction strategies. The proposed model can more objectively support the safety management and risk reduction of natural gas pipelines and other process installations in the digital age.

- **Keywords:** Risk assessment; Natural gas pipeline; Bayesian network (BN); Knowledge graph; DEMATEL

Summaiya Javed, Arun Kumar Tiwari. *Performance assessment of different Organic Rankine Cycle (ORC) configurations driven by solar energy*. Pages 655-666.

This paper deals with the comparison of three Organic Rankine Cycle (ORC) configurations specifically Basic, Recuperative and Regenerative from the energy and economic prospective. Four different organic working fluids (Toluene, Nonane, Decane and Dodecane) are flown individually in all the three configurations. For simulation purpose of various configurations Aspen plus is used, along with energy analysis is done on all the configurations to evaluate the net work done, power and efficiency of ORC systems. As Toluene has zero ozone depletion potential and a low global warming potential, the worry about climatic changes is somehow offset by these beneficial environmental traits. Study shows that the maximum net work done of 1364 kW is given by Regenerative ORC which shows an enhancement of 36.60 % and 25.23 % from Basic and Recuperative ones. Among all the selected configurations and working fluid, Regenerative with Toluene shows the most efficient configuration and gives 37.01 % of maximized efficiency. Along with that the thermo-economic analysis is also performed on all the three configurations out of which Regenerative shows an operating cost of 211.65 $/hr. It is observed that under ideal circumstances the Regenerative ORC along with Toluene working fluid outperforms the other two configurations.'

- **Keywords:** Organic Rankine Cycle; Energy Economic Analysis; Configurations; Parabolic Trough Collector

Hans Langva Skarsvåg, Morten Hammer, Svend Tollak Munkejord, Alexandra Metallinou Log, Stéphane Dumoulin, Gaute Gruben. *Towards an engineering tool for the prediction of running ductile fractures in CO2 pipelines*. Pages 667-679.

A prerequisite for the deployment of CO2 capture and storage (CCS) is to establish a large network of high-pressure transport pipelines. It is then vital to assess new and existing pipeline designs for running ductile fracture (RDF). RDF is a phenomenon in which a defect develops into a crack propagating along the pipeline, sustained by the pressure forces from the escaping fluid. The most common engineering method for RDF, the Battelle two-curve method (BTCM), was originally developed for natural gas (NG) and has proved non-conservative for CO2. In this work we examine the BTCM in the light of available RDF experiments with CO2-rich mixtures. We present an improved material curve, in which the change in fluid properties when replacing NG with CO2 results in a new effective toughness correlation. Furthermore, we present an improved method for calculating the crack-tip pressure. This delayed homogeneous equilibrium model (D-HEM) accounts for the non-equilibrium thermodynamics due to the rapid depressurization, resulting in boiling pressures below the saturation pressure. Together, the adaptation of the material and fluid treatment yields improved results, and is a step towards a viable engineering tool for the prediction of RDF in CO2 pipelines.

- **Keywords:** CO2 pipelines; Running ductile fracture; Carbon dioxide; Decompression; Non-equilibrium; Pipeline integrity

Amol Vijay Sonawane, Z.V.P. Murthy. *Dairy industry wastewater treatment by MOF and 2D nanomaterial engineered PVDF membranes based aerobic MBR: Membrane fouling mitigation and stability study*. Pages 680-693.

In the present research work, PVDF membranes are embedded using zinc imidazolate framework-8 and molybdenum disulfide. The membrane's impact is investigated using their permeability, separation performance, reusability and stability performance and fouling resistance. Results show that the ZIF-8 and MoS2 based PVDF nanocomposite membranes have superior pure water flux performance, such as 27.71 L/m2 h and 32.53 L/m2 h, respectively. The FRR of the ZIF-8 and MoS2-based PVDF nanocomposite membranes is obtained at 95.65 % and 97.04 %, respectively. The flux recovery ratio and water contact angle studies show that prepared membranes have better antifouling performance than pristine PVDF membranes. The pollutant removal performance for COD, BOD5, TN, NH4-N and TP is obtained as 94.08 %, 95.31 %, 94.5 %, 95.56 % and 94.64 %, respectively, from dairy industry wastewater. Also, the microbial culture growth study report that the ZIF-8 and MoS2 based PVDF membranes reject maximum microbes from the treated water. Therefore, the prepared PVDF nanocomposite membranes show outstanding filtration performance, reusability, and long-term stability performance. Hence, the ZIF-8 and MoS2 nanomaterials significantly improved the PVDF membrane's characteristics and could be a promising nanocomposite membrane for practical application in different wastewater treatments.

- **Keywords:** Aerobic process, Nanomaterials; Fouling mitigation; Stability performance; Pollutant removal efficiency, Microbial culture growth

Umair Baig, Abdul Waheed. *Facile fabrication of ceramic-polymeric nanocomposite membrane with special surface wettability using amino decorated NH2-SiO2@SiC nanopowder for production of clean water from oily wastewater*. Pages 694-704.

Given the huge market potential of treating oily wastewater, a ceramic membrane with special surface wettability was fabricated by covalently decorating amino-functionalized silicon carbide (NH2-SiO2@SiC) as an active layer on alumina support. The NH2-SiO2@SiC was synthesized by growing a layer of silicon dioxide (SiO2) on silicon carbide (SiC) leading to silicon dioxide loaded silicon carbide (SiO2@SiC). Then amino (-NH2) functionalization of SiO2@SiC was carried out through 3-triethoxysilylpropylamine (APTES) yielding NH2-SiO2@SiC. The NH2-SiO2@SiC was covalently deposited as active layer on alumina support through interfacial polymerization with terephthaloyl chloride (TPC) leading to SiO2@SiC/polyamide nanocomposite decorated on alumina (SiO2@SiC/PA@Al2O3) ceramic membrane. The SiO2@SiC/PA@Al2O3 ceramic membrane was thoroughly characterized by several membrane characterization techniques including water and oil contact angles, SEM (scanning electron microscopy), elemental mapping, EDX analysis (energy dispersive x-ray) and ATR-FTIR (Attenuated Total Reflectance Fourier Transform Infrared spectroscopy). The SiO2@SiC/PA@Al2O3 ceramic membrane was applied for sepraration of surfactant stabalized oil-in-water (O/W) emulsion feed. The effect of increasing O/W emulsion concentration (33.75–250 ppm) was studied by varying the amount of oil in the emulsion. The ceramic membrane was able to maintain a separation efficiency of > 98 % with permeate flux of 270 L/m2.h at a transmembrane pressure of 2 bar. The long-term filtration tests revealed that SiO2@SiC/PA@Al2O3 ceramic membrane retained its separation efficiency at > 98 % for 420 min when 125 ppm O/W emulsion was used as feed. The SiO2@SiC/PA@Al2O3 ceramic membrane showed a potential of treating a high concentration (250 ppm) surfactant stabalized O/W emulsion.

- **Keywords:** Ceramic membrane; Oil/Water emulsion separation; Silicon carbide; Superhydrophilic; Underwater superoleophobic; Surfactant stabilization

Elayappan Tamilalagan, Muthumariappan Akilarasan, Shen-Ming Chen, Mani Govindasamy, Kuan-Yu Lin, Fatimah Mohammed Alzahrani, Norah Salem Alsaiari. *Construction of perovskite structured ZnSnO3 embedded graphene oxide nanosheets for in-situ electrochemical quantification of organoarsenic roxarsone*. Pages 705-716.

4-hydroxy-3-nitrophenylarsonic acid (HNPA) is an organoarsenic drug commonly known as roxarsone, which has been intensively used as a feed additive in poultry industries. However, the HNPA can easily degrade into highly toxic inorganic arsenic poisoning in biotic and abiotic nature, which threatens human health and the environment. Along with various conventional techniques, the electrochemical sensor based on nanomaterials has emerged as a potential tool for analyzing organoarsenic chemicals, owing to its ease of operation and accuracy. Herein, for the first time, we report the efficient and tremendously sensitive perovskite-structured ZnSnO3@GO nanocomposites for the electrochemical analysis of HNPA. The as-prepared ZnSnO3@GO nanocomposites with good chemical stability, excellent electron mobility, and larger specific area are beneficial to the HNPA reduction. In addition, the analytical performance of the developed sensor shows the minimized reduction potential of (−0.63 V vs Ag/AgCl) with an admirable linear range of 0.01–453.4 μM and a lower detection limit of 0.0043 μM toward HNPA detection. Finally, the real sample analysis of the developed sensor was quantified in the chicken and soil samples, which exhibits appreciable accuracy. The developed ZnSnO3@GO/GCE provides a powerful tool for the rapid and sensitive detection of HNPA in actual samples.

- **Keywords:** ZnSnO3 @GO nanocomposite; Carbon composites; Perovskite structure; Roxarsone detection; Food analysis; Electrochemical sensor

Lin-Quan Gong, Jia-Jia Jiang, Jun-hui Gong, Yong Pan, Jun-Cheng Jiang. *Experimental and numerical simulation study on thermal decomposition model of ammonium nitrate*. Pages 717-725.

High heating rates is one typical character under fire scenario and thermal decomposition behavior of ammonium nitrate (AN) under high heating rates is still unclear. In the current study, a thermal decomposition model of AN was developed to predict thermal decomposition process under high heating rates by a numerical simulation solver Thermakin2Ds based on experimental results. To be more specific, average apparent activation energy and pre-exponential factor were calculated as 75.16 kJ/mol and 3.6×103 s−1 respectively according to simultaneous thermal analyzer (STA) experimental results. Thermal decomposition products were determined as H2O, N2O, NO2, and HNO3 by thermogravimetric-Fourier transform infrared spectrometer (TG-FTIR) experiments. The obtained information was utilized for modelling and determining the most reliable thermal decomposition numerical model of AN. The simulated mass loss and mass loss rate at 10 K/min by the model were accordance with experimental data. The prediction ability was verified at heating rates of 5, 16, 25 K/min. Finally, thermal decomposition processes at higher heating rates of 100, 125, 150, and 200 K/min were predicted. This work is significantly meaningful for the storage safety of AN, providing theoretical guidance for preventing the occurrence of AN explosion from the early fire stage.

- **Keywords:** Ammonium nitrate; High heating rates; Thermal decomposition model; Numerical simulation

Jingshuai Gao, Yina Qiao, Riya Jin, Zengdi He, Jiaoqin Liu, Anlong Wang, Chengjie Guo, Jipeng Mao, MengYe Jia, Xinqiao Feng, Jingjing Zhang. *The treatment of 2,2′,4,4′,6,6′-hexanitrostilbene explosive wastewater by hydrodynamic cavitation combined with chlorine dioxide*. Pages 726-735.

2,2′,4,4′,6,6′-hexanitrostilbene (HNS) explosive wastewater must be strictly treated before discharge due to its a large number of acute toxic mutagenic nitroaromatic compounds (NACs). This study investigated the degradation effect of HNS explosive wastewater by hydrodynamic cavitation combined with chlorine dioxide oxidation (HC+ClO2). The surface-response model was used to simulate the experiment, and it was established that the surface-response polynomial model had high reliability. After the model simulation and experimental investigation, it was concluded that with pH 4.45, ClO2 concentration 14.86 mg/L and treatment time 120 min, the degradation rate of HNS reaches 64.51% in explosive wastewater. Furthermore, the kinetics of HNS degradation by HC or ClO2 oxidation alone and HC+ClO2 oxidation were examined. Compared with the degradation method alone, the degradation effect of HNS by HC+ClO2 was more significant, and the enhancement factor was 1.33, which indicates that HC greatly enhances the oxidation capacity of ClO2. Based on the detection results of the liquid chromatography–mass spectrometry (LC–MS), the possible degradation pathways of HNS were analyzed: within the attack of •OH, HNS were directly or indirectly decomposed into trinitrophenol, after which continuous denitroso occurred to obtain 1,2,3,5-tetrahydroxy benzene, followed by epoxidation cracking to obtain small organic acids, H2O, CO2, etc.

- **Keywords:** Explosive wastewater; LC-MS; HNS degradation pathway; Response surface method; Photoluminescence probe method; Kinetic fitting

Esmaeil Zarei, Faisal Khan, Rouzbeh Abbassi. *How to account artificial intelligence in human factor analysis of complex systems*? Pages 736-750.

Human factors analysis (HFA) has been explored from various aspects (e.g., engineering, psychology, physiology, and ergonomics). Numerous conventional techniques have been developed and applied to improve system safety from the human perspective. However, emerging sociotechnical systems, industry 4.0, and the use of artificial intelligence-driven systems reveal these methods' incapability. This necessity is developing intelligent approaches that account for integrating artificial intelligence (AI) into human factors. This work reviewed the integration of artificial intelligence and expert systems into HFA. It primarily focused on using machine and deep learning and knowledge/data-driven modeling approaches to HFA. Accordingly, this systematic review investigated the applications, contributions, challenges, and research gaps of HFA in complex systems. We analyzed seven vital elements of HFA to illustrate these concerns. This work also highlighted important myths, misapplications, and critical concerns that need to be addressed using advanced approaches.

- **Keywords:** Human error; Human reliability; Human performance; Human factors; Artificial intelligence; Expert systems

Hetang Wang, Jun He, Jinghao Yang, Hui Wang, Yu Zhang, Sisi Cheng, Ziqi Nie. *Cracking and improved wettability of coal through liquid CO2 cyclic cold soaking for dust prevention*. Pages 751-762.

To solve the problem of water injection in low–porosity and low–permeability coal seams, a new idea of liquid CO2 cyclic cold soaking to improve the water absorption and wetting efficiency of coal is proposed. The evolution of the pore structure and mechanical properties of coal were studied using low–field nuclear magnetic resonance and uniaxial compression tests. The wettability and water absorption of coal before and after the experiment were determined using contact angle and water absorption tests. The results show that as the number of cycles increases, the effective porosity of coal increases significantly, the mechanical strength is weakened, and the compressive strength and elastic modulus decrease. The wettability and water absorption of coal samples were significantly improved by liquid CO2 treatment, and the changes in porosity, mechanical strength, and water absorption wettability of coal samples in the saturated group were more obvious compared to dry coal. This paper lays a theoretical and experimental foundation for the development of a new technology for coal seam water injection dust prevention.

- **Keywords:** Coal seam water injection; Dust prevention; Cyclic cold soaking; Pore structure; Mechanical strength; Water absorption

Xun Jia, Yalan Zhang, Guizhou Xu, Xueyao Wang, Ying Liang, Aimin Li, Xianchuan Xie, Daishe Wu. *A novel Bi2WO6/DMPBP composite for cyclic adsorption and photocatalytic degradation of organic pollutant in water*. Pages 763-772.

The typical photocatalyst Bi2WO6 (BWO) has low energy efficiency due to its low specific surface area (SSA) and high photogenerated electron/hole recombination rate. In this study, a three-dimensional spherical BWO/DMPBP[5] composite was synthesized by loading DMpillar[5]arene-based porous polymer (DMPBP[5]) on BWO through hydrothermal method to correct these deficiencies. Scanning electron microscopy and transmission electron microscopy showed that the modified BWO transformed into three-dimensional spherical composite. Furthermore, BET surface area analysis further proved that compared with the original photocatalyst BWO whose SSA is 19 m2·g−1, the

optimized composite BWO-7% exposes more SSA with a value of 134 m2·g−1, endowing it more adsorption and photocatalytic active sites. Results showed that photocatalytic reaction rate constants of BWO-7% increased by more than 10 times, compared with that of BWO. This significant improvement was due to the introduction of DMPBP[5], which could concentrate organic pollutants, thus reduce the distance between contaminants and the active site. More importantly, after DMPBP[5] was loaded, BWO/W5O14 heterojunction was formed. In the detection process, we found that oxygen vacancy was introduced in it, which was more conducive to the separation of electron/hole pairs and improved the photocatalytic performance of visible light. In addition, the adaptability to inorganic salts, pH and recycling performance of BWO composites were excellent. Altogether, this study provides the possibility for the application of new adsorption-photodegradation materials in photocatalytic water treatment.

- **Keywords:** Adsorption-photocatalytic; DMpillar[5]arene; Oxygen vacancy; Heterojunction; Active species

Henrique Martini Paula. *Insights from 595 tank farm fires from around the world*. Pages 773-782.

This article presents several insights from research of fire incident data from tank farms from around the world, which store products ranging from low flashpoint materials to crude and heavier hydrocarbons. The incidents and information in the database came from over 130 mostly publicly available sources, including technical and news reports. Updating of the database takes place when new studies require analysis of previous incidents. The database contained 595 fire incidents at the time of preparation of this article, and this research has already supported the analysis of the reliability of fire water protection system, hazard identification, and risk assessment for several tank farms. The research provided valuable insights regarding the frequency of tank farm fires, the frequency of boilovers, the frequency of injuries/fatalities, the expected numbers of injuries/fatalities per incident, the frequency of dike fires, the probability of failure of the fire water system, the time to extinguish (TtEx) the fires, the ignition source, and the types of tank roofs. When the database provided sufficient information, these numbers appear as a function of the material or product. The data also allowed plotting TtEx as a function of the (a) time for over a century, (b) tank diameter, and (c) number of tanks on fire.

- **Keywords:** Fire; Explosion; Boilover; Tank; Tank farm; Flammable; Combustible; Quantitative risk assessment; Reliability; Fire water protection system

Yanrong Cheng, Xiaoyan Shu, Mingfen Wen, Yuexiang Lu, Pan Tan, Xirui Lu, Lingshuang Li, Faqin Dong. *Immobilize Nd2O3 as simulated nuclear waste in silicate-apatite glass-ceramics*. Pages 783-793.

The solidification of nuclear waste has far-reaching developmental implications. Nuclear waste management is not only essential for the earth's ecological balance but also can address the increasing depletion of human exploitable resources in the future. Scientists are dedicated to finding a better solidification matrix and ensuring the sustainable development of the nuclear industry in search of alternative energy sources. The present work has fabricated a simulated nuclear waste form using a sintering process of diopside. The results have shown that the Fe element in diopside granite porphyry shows an impact on the amorphization process and mechanical properties of the final waste form. Moreover, the study finds a natural analog in the glassy bulk, i.e. (Ca2Nd8(SiO4)6O2 or (K, Na)Nd9(SiO4)6O2), which can solidify the simulated trivalent actinide of Nd3+. The FT-IR results suggested that the polymerization degree of glass components in waste form decreased initially and then increased with Nd2O3 doping. Q3 unit is considered to be a key component in the waste forms. Finally, the loading capacity of Nd2O3 in waste

form reached 19 wt.%. The waste form has the characteristics of glass-ceramics containing a silicate-apatite structure that is evenly distributed and has a quite considerable prospect for mechanical properties.

- **Keywords:** Solidification matrix; Nd2O3; Glass-ceramic; Diopside granite porphyry; Silicate-apatite

Xiaoning Jia, Cailan Li, Xia Zhao, Miao Xu, Yongjie Cai, Tong Wu, Jing Huang. *The electrical generation and oxidation efficiency of a novel bio-electro-Fenton system*. Pages 794-802.

The inner portion of the reaction device of the bio-electro-Fenton (BEF) system was independently designed to construct dual-chamber bio-electro-Fenton systems to simultaneously degrade tetracycline (TC) and levofloxacin (LEV) in both anode and cathode chambers. The electro-Fenton reaction that degrades LEV wastewater in the cathode is propelled by bioelectric energy generated on-site. With graphite felt as the cathode and anode of the motional bio-electro-Fenton system, an external resistance of 10 Ω, pH of 3 in cathode, a Na2SO4 concentration of 0.07 mol/L, an Fe2+ concentration of 0.1 mmol/L and an aeration rate of 3 * 4.5 L/min, the removal rates of TC, COD, TOC, and NH4+-N within 72 h were 59.6 %, 83.7 %, 74.15 % and 80.1 % in the anode. And the LEV elimination rate was 75.50 % and the mineralisation rate was 68.39 % for 20 mg/L in the cathode within 24 h. The highest power density, current density, and voltage of the motional bio-electro-Fenton system could reach 7.12 W/m3, 636.94 mA/m3, and around 900 mV, respectively, and the maximum voltage could be maintained for over 36 h. Analyzing the system's electron transfer mechanism and proposing potential degradation pathways for tetracycline and levofloxacin.

- **Keywords:** Advanced oxidation process Bio-electro-Fenton Levofloxacin Tetracycline

Yousaf Ayub, Jianzhao Zhou, Tao Shi, Jingzheng Ren. *Process safety assessment of thermal technologies for biomass valorization by numerical descriptive approach*. Pages 803-811.

Process-based safety assessment of biomass thermal valorization technologies including hydrothermal gasification (HTG), pyrolysis, and conventional gasification has been evaluated based on the Numerical Descriptive Logistics Equation (NuD). Process-related data such as temperature, pressure, heat of reaction, and process inventory were collected from the literature for this purpose. The data has been analyzed by using the NuD equations to obtain the process safety total score (PSTS), and then hierarchy of control (HOC) has been applied to propose the strategies for risk mitigation. According to the NuD results, the HTG process has a lower PSTS (210.2) compared with pyrolysis (226.4) and gasification (228.5), and it reveals that HTG is the safest among these three technologies. HTG has the highest score for pressure (60.48) because it has the high pressure (20–25 MPa) process requirement, but the lowest scores for temperature and heat of reaction due to lower temperature operations (374–400 °C) compared with pyrolysis and gasification. The results determined by the NuD have been compared with subjective safety evaluation methods (Process Safety Index Analysis and Inherent Safety Index), and the results of inherent safety index (ISI) are also consistent with that determined by the NuD. Hierarchy of control has been proposed to control and reduce the process risk. As per results, engineering and administrative measures could be drafted for more effective process safety control.

- **Keywords:** Safety Assessment; Process Safety; Quantitative Risk; Risk Control; Biomass valorization

Ren-E. Dong, Su Zhanguo, Ibrahim B. Mansir, Azher M. Abed, Xiangjie Niu. *Energy and exergoeconomic assessments of a renewable hybrid ERC/ORC integrated with solar dryer unit, PEM electrolyzer, and RO desalination subsystem*. Pages 812-833.

In this investigation, a zero-dimensional model of a renewable generation system encompassing a solar-geothermal driven Proton Exchange Membrane (PEM) electrolyzer integrated with Organic Rankine Cycle (ORC), Ejector Refrigeration Cycle (ERC) and Reverse osmosis (RO) unit is expressed with respect to energetic, exergetic, economic, and exergoeconomic points of view. Cooling and heating energies, electricity, distilled water, Hydrogen (H2), Oxygen (O2) are the key products of the mentioned system. In order to acquire the influences of the solar collector numbers, area ratio, and pressure drop of the ejector and working fluid of solar collectors on the efficiency of the hybrid unit, a set of equations were coded in MATLAB and Engineering Equation Solver (EES). The exergy destruction rate, exergy efficiency, and exergy destruction ratio of each subsystem and exergy flow diagram of all subsystems were evaluated in this study. Afterward, the results of the sensitivity analysis were used for multi-criteria optimization in three various layouts that the LINMAP as well as the fuzzy TOPSIS decision makings and Gray Wolf Optimizer (GWO), are considered to get the optimal result. The results have indicated that the main variables analyzed are more affected by the variation in the number of the flat plate solar collector. Besides, in the second optimization scenario, the TOPSIS selects the optimal solution of exergy efficiency and unit exergy cost of the product of 3% and 19.77 $/Gj, while the LINMAP selects 3.001% and 19.80 $/Gj point.

- **Keywords:** Multi-generation system; Solar-geothermal driven ORC-ERC; PEM electrolyzer; Multi-objective optimization; Fuzzy TOPSIS; LINMAP

Gabriela Kuchtová, Petr Herink, Tomáš Herink, Jaromíra Chýlková, Petr Mikulášek, Libor Dušek. *From lab-scale to pilot-scale treatment of real wastewater from the production of rayon fiber*. Pages 834-846.

The subject of our study involved the treatment of real process wastewater from the production of rayon fiber. During the annual monitoring of the production facility, we performed a mass balance of three problematic sources of process wastewater and analyzed them repeatedly. All three sources showed high values of COD = 0.4–30 g/L, TOC = 0.09–7.1 g/L and the concentration of Zn2+ 0.09–0.5 g/L. At a total volume of 1.84 million m3, this represents a significant pollution source for the Elbe River. At lab-scale, we tested a combination of filtration, microfiltration, and oxidation using the Fenton, electro-assisted Fenton, and the electrochemical oxidation methods, both on the plate and newly developed macroporous BDD electrodes on a ceramic substrate, along with the final adsorption of Zn2+ emissions on the strongly acidic cation exchange resin Lewatit Mono plus S108. It was tested in Na+ and H+ cycles. Using an optimized technological sequence, we have achieved a COD reduction of up to 98%, and a TOC reduction of 85%. During the H+ cycle cation regeneration by sulfuric acid, Zn2+ emissions were converted to zinc sulfate that can be recycled in the spinning bath of the production process. The method was verified at a pilot scale.

- **Keywords:** Rayon production; Fenton oxidation; Electro-assisted Fenton oxidation; Macroporous BDD electrodes; Electrochemical oxidation, Zn2+ adsorption

Meiyun Qi, Ping Lin, Qiyu Shi, Huiling Bai, Huan Zhang, Weihuang Zhu. *A metal-organic framework (MOF) and graphene oxide (GO) based peroxymonosulfate (PMS) activator applied in pollutant removal*. Pages 847-858.

Fenton-like reactions based on the peroxymonosulfate (PMS) can efficiently degrade pollutants and have attracted widespread attention. Herein, we reported a facile strategy to synthesize a heterogeneous PMS activator (Zn/Co-MOF@rGO-600) derived from a cobalt-zinc bimetallic metal-organic framework (MOF). The Zn/Co-MOF@rGO-600 was applied as the catalyst for the effective tetracycline (TC) removal during the PMS activation process. The introduction of Zn and the presence of graphene oxide (GO) not only enhanced the yield of the single-atom cobalt (Co0) in the catalyst through the bimetallic synergy but also had a positive effect on adjusting the morphology of the catalyst. The charge transfer resistance (Rct) of Zn/Co-MOF@rGO-600 decreased by 3.15 times after GO modification. The reaction rate constant (k) increased by 14.88 times in the reaction system with Zn/Co-MOF@rGO-600 as PMS activator, the corresponding efficiencies of TC removal and mineralization increased to 91.66 % and 45.04 %, respectively. Density functional theory (DFT) calculation suggested that the bonding energy (Ebon) between PMS and the Zn-Co atom was low enough to − 2.76 eV so that the Zn/Co-MOF@rGO-600 could act as an effective PMS activator. The quenching experiment and the radical spin trap test showed the main generated reactive species were SO4•-, O2•- and 1O2. The presence of SO4•- was the main driving factor for the generation of other radicals such as 1O2 and •OH during the PMS activation process. This research proposes a new reference to fabricate an effective catalyst for PMS activation, which was derived from a bimetallic (Zn/Co) MOFs.

- **Keywords:** Peroxymonosulfate activation; Metal-organic frameworks; Advanced oxidation process; Graphene oxide; Transformation of free radicals; Tetracycline removal

Bo Lv, Xiaowei Deng, Feishuo Jiao, Bobing Dong, Chaojun Fang, Baolin Xing. Enrichment and utilization of residual carbon from coal gasification slag: a review. Pages 859-873.

Coal gasification is a clean and effective method for converting coal into syngas, which is mainly used in fuel and chemical industry. However, the process of coal gasification produces copious amounts of solid waste, that is, coal gasification slag, which is very harmful to the surrounding environment, and then to people's lives and health. The residual carbon is the product of incomplete coal gasification and has high economic utilization value in coal gasification slag. Recovery and utilization of residual carbon is an effective method for the comprehensive treatment of coal gasification slag. This study discusses the current methods of recovering residual carbon from slag, such as the physical, chemical, physicochemical and special separation methods, based on the properties of coal gasification slag, further the advantages and disadvantages of each method are compared. Moreover, the utilization of residual carbon as fuel or for the preparation of materials are discussed in detail. Finally, research and development recommendations for the future study of residual carbon in future are discussed based on existing limitations in the field.

- **Keywords:** Residual carbon; Coal gasification slag; Flotation; Acid treatment; Material utilization

Mehdi Faraji, Majid Saidi. *Experimental and simulation study of peanut shell-derived activated carbon and syngas production via integrated pyrolysis-gasification technique*. Pages 874-887.

Carbonaceous materials are among the most appropriate and widely used materials in the field of energy production, conversion, and storage. According to recent studies, biochar-based catalytic supports and adsorbents have shown great potential in the fields of energy production and the adsorption and storage of various gases due to their adjustable surface chemistry and porosity. In the present study, the pyrolysis of peanut shell to produce activated carbon as a precursor for catalyst support was investigated. Acid washing pretreatment was performed on raw biomass before pyrolysis to remove metals and impurities and reduce the ash content of the biomass. Before pyrolysis, thermogravimetric analysis was performed to determine the temperature range of biomass thermal decomposition. Pyrolysis was carried out at temperatures of 300, 400, and 500 °C to study the effect of pyrolysis temperature on biochar yield. KOH-activation on biochar was followed by subsequent pyrolysis at 650 °C to produce activated carbon. To study the effect of pyrolysis temperature and KOH activation on the structural and physiochemical characteristics of biochar, nitrogen adsorption/desorption and FTIR analyses were conducted. The pore size of the activated carbon surface changed from mesoporous to microporous with increasing the pyrolysis temperature and subsequent KOH activation, and the biochar specific surface area increased from 3.5 to 363.1 m2 g-1. In order to evaluate and optimize the operating conditions of the biochar and syngas production processes on larger scales, the integrated pyrolysis and gasification processes were simulated in Aspen Plus software. The effects of temperature, pressure, and air to biomass ratio on biochar production rate and H2/CO ratio were evaluated. A temperature of 650 °C, a pressure of 1 bar and an air to biomass ratio of 0.1 were selected as optimum operating conditions to simultaneously achieve maximum biochar production and maintain the quality of synthetic gas. The findings of the experimental and simulation sections of this study could provide a useful guide for the industrial-scale production of biochar and activated carbon as a catalytic support in various chemical production processes, as well as a water polutant adsorbent and gas adsorbent for various gas purification and storage processes.

- **Keywords:** Biomass; Biochar; Activated carbon; Pyrolysis; Gasification; Simulation

Yishuai Jing, Tianxin Kang, Peng Hu, Haibo Fan, Feng Teng, Xin Zhao, Jiaming Song. *Surfactant-induced photocatalytic performance enhancement of europium oxide nanoparticles*. Pages 888-894.

Recently, rare earth (RE) elements and their oxides have been attracting more and more attention in the field of photocatalytic degradation. Due to the unique 4 f electronic structure and optical properties, the RE element, europium (Eu), together with its oxides, are often used for surface modification of other photocatalysts. Nevertheless, the photocatalytic degradation property of europium oxide has been rarely reported. In this study, we synthesized Eu2O3 nanoparticles via chemical precipitation and calcination processes, and performed surface modification by using surfactants as polyvinyl pyrrolidone (PVP) and hexadecyl trimethyl ammonium bromide (CTAB). Compared with pure Eu2O3 nanoparticles and those synthesized with PVP, photocatalytic degradation efficiencies of Eu2O3 nanoparticles synthesized with surfactant CTAB for degrading rhodamine B dye demonstrated to be improved by 16% and 12%, respectively. The ultraviolet-visible diffuse reflectance spectra measurements indicate that CTAB can increase the bandgap of Eu2O3 due to the reduction of oxygen defects. Photoluminescence spectra demonstrate that the surfactant would affect the luminescence of Eu3+ and carrier redistribution of energy levels.

- **Keywords:** Eu2O3; Photocatalysis; Surfactant; Degradation; Rare earth materials

Te Ma, Lan Lan, Mohammad Marefati. *Assessment of a new multigeneration system based on geothermal plant and a linear Fresnel reflector-based solar unit: An effort to improve performance*. Pages 896-913.

Recently, the development and exploitation of renewables-driven multigeneration systems can be a sensible solution to reduce the limitations of fossil energies and their negative environmental impacts. The combination of two geothermal and solar energies, in addition to reducing the installation costs of solar systems, can support the efficiency improvement of the geothermal-driven energy systems. In addition, the use of suitable downstream cycles in such energy conversion processes can improve thermodynamic and economic performances. The coefficient of performance offered by a generator absorber heat exchanger-based refrigeration cycle can be higher than that by the ejector and absorption refrigeration processes. A comprehensive thermodynamic-conceptual and exergoeconomic evaluations as well as two-objective optimization on a new geothermal-driven multigeneration system, based Sabalan geothermal wells, has been developed in this paper. The proposed system is able to produce power, heating, cooling, and hydrogen fuel. In the developed configuration the geothermal source is considered as the main source of energy production and a linear Fresnel reflector-based solar unit produces a portion of the required thermal power of the system. Further, a single-flash cycle, a water electrolysis unit (based on alkaline electrolyzer cell), and a generator absorber heat exchanger unit are embedded to generate various forms of energy. The overall outcomes indicated that the proposed system can produce 4.1 MW of electric power, 1.67 MW of heating load and 1.46 MW of cooling load. In addition, the hydrogen production rate of the energy process is equal to 5.75 kg/h. In such a context, the considered process can achieve energy and exergy efficiencies of almost 34.2% and 66.3%, respectively. Based on the optimization findings, the energy efficiency can be improved by approximately 9.75% according to the optimal input data. Additionally, the total product unit cost rate can be reduced by almost 4.3% at the same time. Relying on a parametric analysis, variables affecting the performance of the considered system are identified. The conceptual design of the solar unit is also presented regarding the geographical and climatic data of the desired region.

- **Keywords:** Geothermal source; Solar thermal collector; Generator absorber heat exchanger cycle; Alkaline electrolyzer; Exergoeconomic; Optimization

Qilin Li, Yang Wang, Ling Li, Hong Hao, Ruhua Wang, Jingde Li. *Prediction of BLEVE loads on structures using machine learning and CFD*. Pages 914-925.

Boiling Liquid Expanding Vapour Explosions (BLEVEs) are driven by complex fluid dynamics with expanded vapour and flashed liquid. They may generate strong shock waves that lead to catastrophic consequences to personnel and structures in the vicinity. Despite the great interest in safety management and intensive research efforts, reliable and efficient prediction of BLEVE loads on structures is still challenging in practice. Computational Fluid Dynamics (CFD), based on complex physics formulas, can provide more accurate predictions of BLEVE loads than the traditional empirical and TNT-equivalency approaches, but suffers from high computational costs. Data-driven machine learning models offer efficient surrogates but conventional models, including commonly used multi-layer perceptron (MLP), are suboptimal especially for explosions of complex geometry and in complex environment. In this study, a novel machine learning approach, based on the state-of-the-art Transformer neural networks, is developed for BLEVE loads prediction on an idealised structure in the vicinity of BLEVE. Through extensive experiments and rigorous evaluation, it is shown that Transformer can effectively model the structure-wave interaction, yielding accurate pressure and impulse predictions with less than 14% relative errors, which outperforms widely used MLP (20% error)

significantly. The developed Transformer model is applied to predict critical parameters of BLEVE loads, including arrive time, rise time and duration. The results demonstrate that Transformer can produce an accurate pressure-time history, yielding a comprehensive characterisation of BLEVE loads on structures.

- **Keywords:** Gas explosion; BLEVE; Transformer; Machine learning; Blast wave; Interaction with structures; CFD; Neural networks

Yifan Zhang, Fubao Zhou, Jinshi Li, Jianhong Kang, Chun Liu, Ning Li, Shunlin Pan. *Novel efficient energy saving approach for liquid ring vacuum pump in coal mine gas drainage*. Pages 926-937.

Liquid ring vacuum (LRV) pumps used in the coal mine gas drainage system waste a considerable amount of electrical energy due to the extremely low efficiency, which has been a dramatic limitation over many decades not effectively solved using the conventional structural optimization method. Here a novel approach for drastic improvement of LRV pump efficiency, based on turbulent drag reduction theory, is proposed to reduce the useless energy consumption. Furthermore, a new kind of drag-reducing working fluid (DRWF) for the LRV pump and a supporting closed energy-efficiency system, are developed. Industrial-scale measurements are conducted on the LRV pumps with various models to evaluate the influence of the new DRWF on the overall pump performance. The experimental results show that the new approach can achieve approximately 10% pump efficiency improvement and maximally 21–24% energy-saving rate at an optimum concentration of xanthan gum of 4000 ppm in the DRWF. A cost-effectiveness analysis shows the economic viability of this approach. This technology has been commercially applied to reduce the electricity waste in coal mine gas drainage system, and the energy-saving rate reaches 15–22%, and the carbon emissions reduction for Gucheng mine in China can reach 987 tons per year, which is proved to be an effective approach to achieve China's carbon peak and neutrality goals.

- **Keywords:** Liquid ring vacuum pump; Gas drainage; Performance improvement; Energy saving; Drag reducing fluid

Mohammad Tahmasebzadehbaie, Hoseyn Sayyaadi. *Condensate polishing plant debottlenecking within a combined cycle power plant considering the limitation of water resources*. Pages 938-950.

The most challenging problem with using Heller towers is the lack of proper water cooling in the hot air temperature. This matter creates a problem of increasing the condensate polishing plant’s (CPP) inlet water temperature, which deactivates the power plant cycle. CPP inactivation reduces the cycle water quality and damages the power plant's equipment. In this study, the thermodynamic conditions of a cycle were obtained in different weather conditions by modeling and encoding a combined cycle power plant in Yazd, located in Iran, using Thermoflex and MATLAB software. Then two solution scenarios of the air-cooled cooler and wetted-medium evaporative cooling were considered for debottlenecking of the CPP. The investment cost of the ACC was US $ 82,488, and this scenario could solve the CPP problem totally without using water with a payback period of 0.13 years. Using the water injection method, the annual water consumption was 835027 m3. The reverse osmose desalination and wetted-medium cooling investment costs were also US $ 8757300. This scenario could be used for CPP’s debottlenecking as well as increasing the steam cycle's power generation. This scenario is facing a significant challenge due to the high-water consumption. The Air-cooled cooler was chosen as a better solution by TOPSIS decision-making method. If a small-scale investment is intended to solve the CPP problem, the first scenario is preferable. If large-scale investment with profit from excess electricity generation, solving the CPP problem, and without water-shortage consideration are considered simultaneously, then the second scenario is highly recommended.

- **Keywords:** air-cooled cooler; combined cycle power plant; condensate polishing plant (CPP); Heller dry cooling tower; debottlenecking

Jiang Chenyu, Yang Jun, Xue Ke, He Zhanyu, Yang Ming. *Coupling of adjoint-based Markov/CCMT predictive analytics with data assimilation for real-time risk scenario forecasting of industrial digital process control systems*. Pages 951-974.

isk early detection and controls are critical to avoid unforeseen accidents or incidents across safety-critical industries especially in a digitalization context. Using the sequential Monte Carlo particle filter method, an adjoint-based Markov/Cell-to-Cell Mapping Technique (Markov/CCMT) predictive analytics coupling with data assimilation is proposed in the paper for dynamic risk and reliability scenario modeling of industrial digital process control systems. The particle filter-based data assimilation method is developed with a sequential importance sampling with resampling scheme for extended system state estimation and dynamic reshaping of system state-space model. Then the Markov/CCMT predictive analytics models are dynamically constructed using an equal-weight quadrature scheme for approximating the probabilistic cell-to-cell mapping relations that reflect the possible system state transitions on the discretized state-space model in real time. The adjoint-based Markov/CCMT modeling for risk scenario forecasting is demonstrated on a digital U-shaped Tube Steam Generator (UTSG) water level control system in nuclear power plants. The demonstration results show that super real-time and consistent predictions can be obtained within the adjoint-based Markov/CCMT predictive analytics framework. Multi-step time-series forecasting towards the identification of system-level degradation states and risk-significant scenarios evolution can also be envisioned when a blended state merging and pruning strategy is adopted in deep model search. The proposed Markov/CCMT predictive analytics is able to deliver proactive insights to intelligent operation and maintenance of complex safety-critical engineering systems.

- **Keywords:** Dynamic reliability and risk analysis; Data assimilation; Particle filter; Markov/CCMT; Digital process control systems

Kocherlakota Pritam, Harish Puppala, Sridhar Palla, Dadi V. Suriapparao, Tanmay Basak. *A two-step hybrid multi-criteria approach to analyze the significance of parameters affecting microwave-assisted pyrolysis*. Pages 975-985.

Biomass is a viable alternative to fossil fuels due to the abundant availability of solid waste and the associated greenhouse gas emissions. Various conversion methods, including physical, thermal, biochemical-microbial, and chemical processes, have been utilized to convert biomass to energy. Microwave-assisted pyrolysis (MAP) is one of the prominent techniques to convert biomass into energy. Various parameters affect the yield and quality of the product in MAP. Studies addressing comprehensive insight into all influencing parameters are limited. Moreover, the relative hierarchy of the parameters is not evaluated in any of the past research works. Considering this limitation, this study proposed a two-step approach based on a multi-criteria technique that aid stakeholders to analyze the significance of each parameter. The proposed approach is built on the theory of Fuzzy Delphi and the Analytical Hierarchy Process. A total of 27 different parameters affecting MAP are identified through extant literature. Analysis based on the proposed approach suggests that microwave power is the most significant parameter influencing MAP. The impact of co-processing feedstock is very minimal among all the identified parameters. The relative hierarchy of all the parameters drawn in this study help stakeholders performs MAP with the least resources.

- **Keywords:** Biomass; Microwave-assisted pyrolysis; Multi-criteria analysis; Overall dominance; Fuzzified score

Mikail Olam, Hüseyin Karaca. *Optimization of process parameters at direct liquefaction of waste PETs*. Pages 986-994.

Waste polyethylene terephthalate (wPET) was converted to liquid fuel by direct liquefaction method. Additionally, how the catalyst (sodium borohydride) and microwave pre-treatment affect the total conversion and the char yield were investigated. Direct liquefaction experiments were carried out in a batch reactor under non-catalytic/catalytic conditions, and reaction temperature of 325–425 °C, and solid/solvent ratio of ¼, and reaction time of 15–90 min, and microwave pre-treatment time of 3–10 min, and an initial nitrogen pressure of 20 bar. Both the microwave pre-treatment and sodium borohydride (NaBH4) increased the total conversion in the direct liquefaction of wPETs. According to fourier transform infrared spectroscopy (FTIR) and X-Ray diffraction (XRD) analysis of char samples obtained in the direct liquefaction process, the NaBH4 was converted to sodium borate (Na2B8O13). NaBH4 made both hydrogen (H) donating and catalytic effect. The highest total conversion in direct liquefaction of wPETs, which has at the reaction time of 30 min, and the reaction temperature of 400 °C, and in presence of NaBH4, and the microwave pre-treatment of 3 and 8 min, was 62%. The optimum process parameters in direct liquefaction of wPETs are the reaction time of 30 min, and reaction temperature of 400 °C, and the microwave pre-treatment time of 3 min.

- **Keywords:** PET recycling; Sodium borohydride; Direct liquefaction; Microwave pre-treated; Process parameters; Total conversion; Char and oil yield; Characterization

Xulei Hou, Hao Lan, Ziming Zhao, Jianwei Li, Chenshu Hu, Yuejuan Li. *Effect of obstacle location on hydrogen dispersion in a hydrogen fuel cell bus with natural and mechanical ventilation*. Pages 995-1008.

Hydrogen leakage in hydrogen fuel cell buses can cause danger to the public. Cuboid space finite element models are established to study the effect of obstacle positions on the hydrogen dispersion behaviour under no ventilation, natural ventilation and mechanical ventilation by monitoring the hydrogen concentration along the line and on the iso-surface. The effect of the obstacle on the hydrogen dispersion behaviour is enhanced with the reduction of the distance from the obstacle to the leakage location. In the space with no ventilation, the effect of the obstacle on hydrogen dispersion varies with the dispersion phase. In the naturally ventilated space, the concentration of hydrogen on the side with an obstacle is higher than that on the side without any obstacles; thus, the presence of the obstacle is not conducive to hydrogen exiting the compartment. In the mechanically ventilated space, the effect of the obstacle on hydrogen dispersion is more pronounced. Specifically, the hydrogen concentration on the side with no obstacles is 2–3 times that on the side with an obstacle, so the obstacle is conducive to hydrogen exiting. The obstacle is recommended to be in the focus of the related hydrogen leakage behaviour study.

- **Keywords:** Hydrogen leakage; Obstacle; Dispersion; Natural ventilation; Mechanical ventilation

Ningjie Sun, Zhe Wang, Yuan Li, Bolin Sun, Zhancheng Guo. *A new technology on continuous purification of galvanized zinc liquid through supergravity-induced filtration*. Pages 1009-1021.

The removing of suspended dross in galvanized zinc is the key point to obtain defect free coatings and inhibit the generation of solid wastes including surface and bottom dross

which are detrimental to preserving environment. A supergravity technology was used to induce the galvanized zinc liquid to be purifying through ceramic foam filter (Al2O3 CFF). Al-Fe intermetallic were the dominant inclusions and precipitated in the galvanized zinc liquid as suspended dross. During the processing of purifying galvanized zinc liquid, inclusions were intercepted on the surface of Al2O3 CFF as residue by the way of being wrapped in oxide film, and some fine inclusions were captured in the filter. The removal ratio of Fe (RFe), loss percentage of Al (LAl) and the yield of zinc (YZn) respectively reached 76%, 63% and 96% at T = 450 °C and G= 50 through the Al2O3 CFF with pore size of 170 ppi and thickness of 20 mm. According to the exploratory experiment on the purification, a continuous purification was further performed for completing engineering scale purification of galvanized zinc liquid. RFe of 73% and LAl of 59% were obtained after the process of continuously purifying 8 kg molten galvanized zinc.

- **Keywords:** Galvanized zinc; Defect-free coatings; Separation efficiency; Supergravity; Engineering scale

Francesco Di Maio, Stefano Marchetti, Enrico Zio. *A framework of sensitivity analysis for the performance assessment of safety barriers impacted by NaTech accidents*. Pages 1022-1030.

Hazardous Natural events can cascade into Technological accidental scenarios (so called NaTech accidents). The occurrence of these accidents can degrade the performance of the preventive and mitigative safety barriers installed in the technological plants. Such performance degradation is typically assessed by expert judgement, without considering the effect of the magnitude of the natural hazard, nor its increasing frequency of occurrence in view of climate change. In this work, a novel sensitivity analysis framework is developed to identify the safety barriers whose performance degradation is most critical and thus needs careful modeling for realistic risk assessment. The framework is based on the calculation of a set of sensitivity measures, namely the Beta, the Conditional Value at Risk (CVaR) and the Value of Information (VoI),●and their use to prioritize the safety barriers with respect to the need of:●accounting for performance degradation during an accidental scenario;●planning investments for further characterization of the safety barrier performance.An application is shown with respect to a case study of literature that consists of a chemical facility equipped with five safety barriers (of three different types, active, passive and procedural). NaTech scenarios can occur, triggered by floods and earthquakes. The results obtained with the Beta measure indicate that two-out-of-five barriers (one active and one passive) deserve accurate modelling of the performance degradation due to natural events. An additional outcome is that in the case study considered, both CVaR and VoI rank the passive barrier as the most effective in mitigating the scenarios escalation: therefore, this barrier is the one for which the decision maker could decide to invest resources for improving the characterization of its performance to obtain a more realistic assessment of the risk.

- **Keywords:** NaTech; Safety barriers; Sensitivity analysis; Value of Information; CVaR; Beta measure

Vicente Elício P.S.G. da Silva, Silvio Luiz de Sousa Rollemberg, André Bezerra dos Santos. *Step-feeding in aerobic/anoxic cycles enhanced the performance of aerobic granular sludge (AGS) systems treating effluents with low C:N ratios*. Pages 1031-1042.

Aerobic granular sludge (AGS) systems treating effluents with a C:N:P ratio similar to real old landfill leachate were evaluated on simultaneous C, N and P removals, and to reduce the main problems encountered, such as nitrite accumulation, biomass loss, and granule disintegration. Therefore, six sequential batch reactors (SBR) were operated with different anaerobic (A), anoxic (An), and aerobic (O) configurations: A/O (R1 and R2),

O/An with conventional feeding and well-defined anoxic phase (R3), O/An with step-feeding and well-defined anoxic phase (R4), and O/An (R5 and R6). The O/An with step-feeding reactor (R4) had the highest biomass retention/settleability (SVI30 < 50 mL/g), the best nitrification rates (99%), and chemical oxygen demand (COD) (97%), total nitrogen (91%) and total phosphorous (55%) removals. Furthermore, there was no nitrite accumulation, and granules' disintegration was insignificant. The most abundant phylum in the reactors O/An was Planctomycetota, composed mainly of organisms from the Pirellulaceae and Legionellaceae families. In these reactors, the abundance of phosphorus-accumulating organisms (PAOs) and denitrifying bacteria were similar, while the abundance of glycogen-accumulating organisms was much higher than PAOs. Therefore, the type of cycle directly influences performance, granule characteristics, and system stability, being important for future investigations applying the AGS technology to leachate treatment.

- **Keywords:** Landfill leachate; Aerobic granules; Engineering aspects; Cycle optimization; Feeding strategies; Microbial community composition