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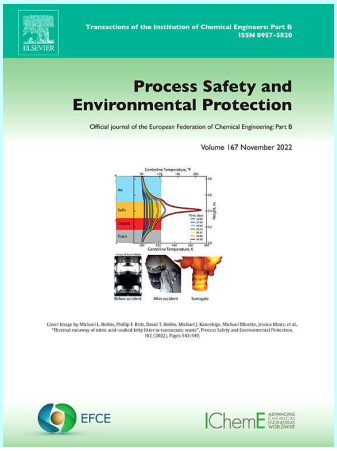

İsmail Şimşek, Levent Altaş. *A fast and effective method for ammonium removal: Emulsion Liquid Membrane*. Pages 1-11.

In this study, ammonium was removed from an aqueous solution by using the Emulsion Liquid Membrane technique. The optimum values of the parameters that had effects on the removal process were determined and results were analyzed using statistical methods. As a result of the conducted experiments, it was determined that the volumetric ratio of the emulsion phase was 0.12, the effective internal phase source was H2SO4, the internal phase volumetric ratio was 0.42, the internal phase concentration was 0.36 N, the surfactant ratio was 2 %, the diluent ratio was 34/64 (mineral oil/toluene, %, v/v), homogenizer speed and time were 10,000 rpm and 1 min, agitation speed was 250 rpm, and external phase pH was 10.80. The fact that 98 % yield was achieved in a very short extraction time (15 s) under optimal conditions and the fact that the studies conducted on this subject in the literature are limited and different reveals the importance of this study obviously.

- **Keywords:** Ammonium removal; Emulsion liquid membrane; Wastewater treatment; Ammonia extraction

Bisham McCarthy-Singh, Alberto Gambaruto. *Experimental and numerical modelling of pressure piling using homogeneous explosive mixtures*. Pages 12-20.

The design of electric valve actuators for explosion proof (Ex d) hazardous environments, whereby an explosive event must be contained, is examined in this study. Combustion within these small enclosed volumes is complex due to the irregular geometries developed in the design process, effectively producing a series of obstacles. These geometries lead to a scenario whereby combustion within the enclosed interconnected volumes produces the phenomenon known as pressure piling. A numerical method utilising OpenFOAM (Foundation), an open-source computational fluid dynamics (CFD) code, has been developed to simulate combustion within two interlinked vessels. OpenFOAM has not been validated extensively for simulating pressure piling. The

numerical results are in good qualitative and quantitative agreement with a set of experimental data. A unique experiment conducted by the author, which introduces obstacles representing blockage ratios (BR's) is presented. Understanding the mechanisms of pressure piling will eventually lead to improved design techniques to control the effects of the over-pressures produced by these types of internal geometries.

- **Keywords:** Pressure piling; OpenFOAM; Closed interconnected vessels; Gas explosion

Oguz Arslan, Asli Ergenekon Arslan. *Performance evaluation and multi-criteria decision analysis of thermal energy storage integrated geothermal district heating system*. Pages 21-33.

Geothermal energy use in district heating systems has been prevalent and familiar in areas with rich sources for many years. In conventional geothermal district heating systems (GDHS), the geothermal fluid is transported to a heat center to give its heat energy to the secondary fluid. Then, this secondary fluid is circulated in the city network to give its heat energy to the heating circuit by the heat exchangers in the substations. Finally, the geothermal fluid is re-injected to handle the continuity of the resources. This current system works under the designed conditions of a heating system with significant electricity consumption and enormous heat waste. In this study, a thermal energy storage (TES) system was integrated into substations instead of heat exchangers to prevent the waste of heat and overconsumption of electricity by obtaining just-in-time working conditions. In this regard, a shell and tube latent heat TES system was designed for residential use for peak loads and integrated into the heating circuit of GDHS, preserving the current main structure. A number of 37 available cases were formed parametrically to evaluate the system's performance. These cases were analyzed thermodynamically by energy and exergy methods. The net present value (NPV) method was used to evaluate the cases' economics. Finally, an efficiency analysis technique with output satisficing (EATWOS) was conducted to determine the most efficient design from the viewpoints of exergy efficiency, NPV, and CO2 emissions.

- **Keywords:** Efficiency analysis; Exergy analysis; District heating; Geothermal; Thermal energy storage

Pallavi Kumari, Syeda Zohra Halim, Joseph Sang-Il Kwon, Noor Quddus. *An integrated risk prediction model for corrosion-induced pipeline incidents using artificial neural network and Bayesian analysis*. Pages 34-44.

In onshore hazardous liquid transmission pipelines, corrosion-induced incidents are potentially significant hazard to people, property and environment. Therefore, several statistical data analysis methods have been developed to analyze their risks. These existing models utilize only a few attributes from a wide incident database and generally assume failure rates as homogeneous or constant over time which is not true. There is also a lack of frameworks to predict risk by utilizing the current condition of pipelines and historical incident data simultaneously. This article presents an integrated risk prediction model which leverages rich incident database of Pipeline Hazardous Material Safety Administration (PHMSA) and utilizes nonhomogeneous failure rates derived from data. From incident data for 2010–2019, 70 attributes are selected based on their significance to corrosion-induced pipeline incidents, and artificial neural network (ANN) models are developed for the prediction of causes and consequences of incidents. Next, the probability of incident is predicted using Bayesian analysis with nonhomogeneous failure rates. Here, ANN models employ current conditions of pipelines and Bayesian analysis utilizes historical incident data simultaneously. The predicted consequences and

probability are multiplied to predict risk of corrosion-induced incidents. The effectiveness of the proposed framework is demonstrated using the PHMSA database.

- **Keywords:** Pipeline incidents; Risk analysis; Artificial neural network; Bayesian analysis

Jianwei Cheng, Yongzhen Ma, Weidong Lu, Guozhong Liu, Feng Cai. *Using inverting CO critical value to predict coal spontaneous combustion severity in mine gobs with considering air leakages – A case study*. Pages 45-55.

The mined-out space in underground coal mines increases due to the mining face advances. The airflow continuously could enter the mine gob via the air leakage channels, which may cause the coal in gob spontaneously ignite and combust. The gob is not accessible for personal direct gas composition measurement due to rock collapses and blockages. Thus, it is difficult to monitor its spontaneous combustion condition timely, which leads to the blindness of developing spontaneous combustion prevention measures. Therefore, it is important to understand the status of spontaneous combustion of residual coal in the gob in time. To more accurately predict the coal spontaneous combustion in gobs, this paper proposes a new model to predict the burning state of coal in the gob by using the gas-CO generated by coal spontaneous combustion with considering the action of air leakages in the gob. Then the reflected CO critical value in the corner of the longwall face in return airflow side can be derived. An example application is also presented in this paper, which shows that the proposed method could better reflect the spontaneous combustion state of gob, and the derived critical value can be used as an early warning message to prevent the coal spontaneous ignition in the gob and reduce the probability of coal spontaneous combustion accidents.

- **Keywords:** Coal spontaneous combustion; Three zones; Temperature-programmed experiment; Backwind corner in longwall faces; Prediction model

Monu Verma, Rupam Borah, Ashwani Kumar, Seon-Ha Chae, Shu-Yuan Pan, Vinod Kumar, Mikhail S. Vlaskin, Hyunook Kim. *Capturing of inorganic and organic pollutants simultaneously from complex wastewater using recyclable magnetically chitosan functionalized with EDTA adsorbent*. Pages 56-66.

Herein, we synthesized new and versatile magnetite-doped chitosan−ethylenediaminetetraacetic acid (Fe3O4@CS−EDTA) composite for simultaneous capturing of multiple heavy metal ions: Hg2+, Cd2+, and Ni2+, and methyl orange (MO) dye from complex wastewater through adsorption process. We believe that EDTA in the synthesized adsorbent works as a cross-linker as well as a chelating agent for the capturing of heavy metal ions, while the protonated amino groups of CS capture MO through electrostatic interaction. In the monocomponent system, the adsorption followed to Langmuir model and gave the maximum adsorption capacities of 232.70 ± 14.30, 121.40 ± 7.0, 56.50 ± 2.20, and 732.10 ± 72.40 mg g−1 for Hg2+, Cd2+, Ni2+, and MO, respectively. Kinetics data well fitted to the pseudo-second order (PSO) models, confirmed the chemisorption process. Interestingly, in the case of the binary component system containing both metals and MO, the adsorption capacity of the adsorbent for the dye was not affected by metal presence, while the adsorption of metal ions was enhanced with increasing MO concentration. The adsorption mechanism was confirmed by elemental mapping, XPS and FTIR. Moreover, no significant loss in the adsorption efficiency even after the six continuous adsorption-desorption cycles confirms the great stability and potential of the adsorbent in treating the complex wastewater.

- **Keywords:** Binary system; Chitosan polymer; Complex wastewater; Multiple pollutants; Synergetic effect

Yunfei Ma, Jianbing Wang, Huijiao Wang, Chunrong Wang, Can He, Xian Zhang. *Performance and integrated mathematical simulations of catalytic ozonation of dimethyl phthalate with activated carbon in continuous gas-liquid-solid reactors*. Pages 67-76.

How to predict the efficacy of heterogeneous catalytic ozonation reactors in reducing pollutants remains limited by complex multiphase systems. An integrated mathematical model of catalytic ozonation by activated carbon (AC) was developed based on hydrodynamics, mass transfer, adsorption, and reaction kinetics to simulate the performance of gas-liquid continuous flow catalytic ozonation reactors. A novel method was proposed reflecting the catalyst behavior to transform the complex gas-liquid-solid multiphase catalytic system into mass conservation equations for each component in gas and liquid phases. The catalyst activity is assumed to be mainly represented by adsorption and the transformation of ozone to hydroxyl radicals (•OH) by active groups on catalyst surface. A mathematical formulation of •OH generation was derived based on the Langmuir-Hinshelwood (LH) mechanism. The model simulation results obtained the concentration profiles of each component and achieved a satisfactory predictive power with error less than 20%, which in turn justified the modeling process. Sensitivity analysis showed that parameters including gas-liquid mass transfer coefficient, secondary reaction rate constant for indirect oxidation and catalyst capacity transfer coefficient have greater influence on simulation results. The optimal conditions for ozone utilization and pollutant degradation were obtained using the validated model simulations: catalyst dosage of 5 g/L, gas flow rate of 0.05 L/min, and initial ozone concentration of 50 mg/L. The results suggest that this mathematical model can provide useful information for design and optimization of catalytic ozonation reactors during industrial applications.

- **Keywords:** Catalytic ozonation; Modeling; Continuous reactors; Hydroxyl radical; Performance analysis

Jingxin Liu, Hang Jia, Meng Mei, Teng Wang, Si Chen, Jinping Li. *Efficient degradation of diclofenac by digestate-derived biochar catalyzed peroxymonosulfate oxidation: Performance, machine learning prediction, and mechanism*. Pages 77-88.

Diclofenac (DCF), a widely used drug, is frequently found in natural waters, and its removal has caused extensive concern. Sulfate radical-based advanced oxidation processes are efficient for the degradation of organic pollutants, but the self-decomposition of persulfates is always sluggish and restricted. Herein, self-N doped biochar derived from food waste digestate (FWDB) was evaluated as the activator of peroxylmonosulfate (PMS) in terms of DCF degradation. The effects of several key operating variables were examined, and the results indicated that ~93% of DCF with an initial concentration of 20 mg/L was removed at FWDB dosage of 0.3 g/L and PMS concentration of 1.0 mM. Thereafter, the machine learning method was explored to simulate and predict the DCF removal process. The reactive oxygen species participated in the reaction was identified as 1O2, and the reaction sites on FWDB were determined as graphitized carbon, CO structure, doped-N, and defective edges. Moreover, based on the identification of intermediates and products, the possible DCF destruction pathways were proposed as hydroxylation, cleavage of N−C bond, and decarboxylation. This study provided an economical and convenient heterogeneous PMS activator for remediation of organic wastewater and confirmed the feasibility of optimizing the contaminant degradation process via data mining.

- **Keywords:** Diclofenac removal; Self-N doped biochar; Peroxylmonosulfate activation; Support vector machine; Degradation pathways

Shuyu Hu, Ao Feng, Jihao Shi, Junjie Li, Faisal Khan, Hongwei Zhu, Jian Chen, Guoming Chen. *Underwater gas leak detection using an autonomous underwater vehicle (robotic fish)*. Pages 89-96.

Gas leaks from subsea oil and gas facilities could cause significant ocean environment damage. Such leaks can cause fire and explosion, for example, a fire on the ocean surface west of Mexico's Yucatan peninsula. Detecting a gas leak is critical in managing fire and explosion risks. This study proposes using autonomous underwater vehicles - robotic fish- for gas leak plume detection. The robotic fish is equipped with advance two well-known deep learning models, Faster RCNN and YOLOV4. A physical experiment system of various sizes of underwater gas leaks is used to generate the benchmark dataset. The results demonstrated the YOLOV4 model has a stronger online real-time capability. It is 43 times faster than the Faster RCNN model with the same level of accuracy. This study verifies the feasibility of integrating deep learning models with the mobile vehicle for real-time autonomous gas leak detection. This contribution will enable the development of a safe and reliable digital twin of subsea emergency management.

- **Keywords:** Autonomous underwater leak detection; Deep learning; Robotic fish; Jetson Nano; Artificial Intelligence; Physical dataset

Guorui Zhang, Enyuan Wang, Chaolin Zhang, Zhonghui Li, Dongming Wang. *A comprehensive risk assessment method for coal and gas outburst in underground coal mines based on variable weight theory and uncertainty analysis*. Pages 97-111.

Coal and gas outburst is one of the main disasters that seriously affect the underground safety production of coal. It is crucial to accurately assess the risk level of coal seam outbursts under different conditions and take effective prevention and control measures to avoid the occurrence of such disasters. To solve this problem, a new assessment method combining variable weight theory and unascertained theory is proposed. Based on qualitative and quantitative risk factors, eight indicators and four classification criteria are constructed. The constant weights (CW) are determined by the fuzzy analytic hierarchy process, while the variable weights (VW) of different parameters by constructing a partitioned variable weight model through the VW theory. Meanwhile, four membership functions of linear (L), parabolic (P), S, and Weibull (W) are proposed to measure the uncertainty level of risk. Based on the calculation of 45 sets of sample data, the differences between the maximum membership principle and the confidence criterion in risk identification were considered, and the optimal hybrid model for the risk evaluation of underground coal seam outburst was derived as VW-P-M. The reliability of the model was determined by further validation of the field data. Finally, the limitations of traditional identification approach are analyzed and the stability of the model under various indicators changes is examined with global sensitivity analysis (GSA). The model fully considers the uncertainty in the outburst risk assessment and the influence of index parameters change on the weight. In addition, it can well solve the risk misjudgment problem caused by low indicators parameters in the production process, providing a reasonable idea and method for the accurate assessment of outburst risk in the early stage of coal mining.

- **Keywords:** Coal and gas outburst; Risk assessment; Variable weight theory (VW); Unascertained measurement (UM) ; Global sensitivity analysis (GSA)

Steffi Talwar, Anoop Verma, Vikas Kumar Sangal, Urška Lavrenčič Štangar, Mika Sillanpää, Ahmed A.S. Al-Othman. *Application of once-*

***through plug flow reactor in the fixed mode for the treatment of pharmaceutical drug-Phenazone using waste-driven visibly active composite*. Pages 112-125.**

In the present study, a low-cost visibly active Fe-TiO2 composite was prepared using waste material for the degradation of Phenazone (PHZ) a pharmaceutical drug using a once-through plug flow reactor. The reactors in the series model were employed and their performance was evaluated using analysis of RTD and was further optimized and cross-checked using BBD. The hybrid process was facilitated by the use of a composite material produced using natural fuller's earth and foundry waste sand (both natural sources of iron) with a TiO2 layer on the outer surface. Analysis suggested a hybrid process in which •OH from both processes are generated simultaneously, which contributes to faster removal. The best possible optimized conditions for three reactors in series were obtained at a flow rate of 10 L h−1, H2O2 dosage of 200 mg L−1, and 80% exposed surface area to achieve the maximum removal of PHZ. The retaining of hybrid catalytic activity under critical flow conditions, even after 250 recycles, verifies its credentials for handling real conditions. The application of composite materials through PFR broadens understanding of the hybrid process of photocatalysis and photo-Fenton on large scale at affordable costs for degradation of various contaminants.

- **Keywords:** Reactors in series; Once through; Fuller's earth; Foundry Sand; RTD analysis; Photocatalysis; Photo-Fenton; Phenazone degradation

Wei Wei, Jian-jun Su, Feng-lei Huang. *Development of pressure-impulse diagram to predict the damage of simply supported RC beams under close-in explosion*. Pages 126-145.

This paper develops the pressure-impulse (P-I) diagram to conduct damage assessment of simply supported reinforced concrete (RC) beams under close-in explosion based on the equivalent single-degree-of-freedom (SDOF) model. Firstly, eleven close-in explosion tests are carried out with different charge weight, scaled distances and offset distances of explosives relative to the mid-span of RC beams. Test results show that the maximum rotation angle can characterize the comprehensive spalling/bending damage under asymmetric load, therefore it is selected as the damage criteria. Then, the equivalent SDOF model is improved by considering the influence of asymmetric load on flexural resistance, and is verified through the test results. Both test results and SDOF model show that increasing the offset distance results in asymmetric bending failure and reduces peak deflection. Through comparative analysis, the equivalent uniform load is chosen to be the axis of P-I diagram. The asymptotes and shape parameters of P-I curves are related to the offset distance and load uniformity. The relationship is derived through curve fitting and validated with the test results and the calculated results of SDOF model. This work expands the application scope of P-I diagram, which contributes to a more comprehensive damage assessment of RC structures under close-in explosion.

- **Keywords:** Damage assessment; SDOF model; P-I diagram; Close-in explosion; Asymmetric load

Hadi Esmailzadeh, Roonak Daghigh, Hamid Khayyam. *Integrated Kalina cycle in a combined polymer membrane fuel cell and evacuated heat pipe collector for a new power generation system*. Pages 146-161.

This paper presents the integration of the Kalina cycle process in a combined polymer membrane fuel cell and evacuated heat pipe collector for improvement of power generation efficiency. The proposed system is evaluated from thermodynamic, environmental, and exergoeconomic perspectives, and the effect of key system parameters are investigated. The energy and exergy efficiencies of the proposed system

in the given conditions are improved by 13.12% and 10.35%, respectively compared to an independent fuel cell. The system's product unit cost of the system and output power in this condition are 136.1 $/GJ and 145.1 kW. The system also prevents the production of 116.1 kg/hr of carbon dioxide under these conditions. The analysis of system parameters shows a direct relationship between increased current density, temperature, and operating pressure of the fuel cell and decreased energy and exergy efficiencies. On the other hand, the total product unit cost increases as these parameters increase. The system assessment shows there is a suitable turbine inlet pressure to achieve optimal efficiency, the lowest unit price for the product, and maximum CO2 emission reduction. Although solar collectors reduce the system's energy efficiency, they increase the exergy efficiency and reduce the cost per unit of the total product.

- **Keywords:** PEM fuel cell; Solar energy; Kalina cycle; Evacuated heat pipe; Exergoeconomic; Waste heat recovery

Zengkai Liu, Qiang Ma, Xuewei Shi, Qi Chen, Zhonghao Han, Baoping Cai, Yonghong Liu. *A dynamic quantitative risk assessment method for drilling well control by integrating multi types of risk factors*. Pages 162-172.

Drilling well control is complex and dynamic with high uncertainty because of the complicated geological conditions and operational environments. Until now, quantitative risk assessment on drilling well control is not integrating human errors, equipment failure, and internal mechanisms together. To address the research gap, this paper presents a novel dynamic quantitative risk assessment method for drilling well control by integrating multi types of risk factors. The entire dynamic Bayesian network is composed of models of human factors, mechanical factors, and environmental factors. The presented method is demonstrated by a case of well section. The dynamic characteristics of the overall risk and individual risks caused by different types of factors are obtained. The influences of human, mechanical and environmental factors on drilling well control risk are researched. It shows that environmental factors have the highest influence on the whole drilling well control risk in Breccia formation. The parameters uncertainty analysis on collapse pressure and fracture pressure of three different rock formations are carried out. It is found out that in-situ stresses have the highest influence on the collapse and fracture pressure.

- **Keywords:** Quantitative risk assessment; Drilling safety; Dynamic Bayesian network; Parameter uncertainty

Qingxiang Shu, Zhenhua Sun, Ganyu Zhu, Chenye Wang, Huiquan Li, Fang Qi, Qikun Zhang, Shaopeng Li. *Highly efficient synthesis of ZSM-5 zeolite by one-step microwave using desilication solution of coal gasification coarse slag and its application to VOCs adsorption*. Pages 173-183.

The increased production of coal gasification coarse slag (CGCS) has placed a significant environmental load on the environment. In this research, one-step microwave synthesis employing coal gasification coarse slag desilication solution as the major source of Si and Na increased the nucleation and crystallization rate of ZSM-5 zeolite. The optimum synthesis conditions were 180 °C, 4 h, Na2O/SiO2 molar ratio of 0.2, and SiO2/Al2O3 molar ratio of 200, which led to a relative crystallinity of ZSM-5 zeolite higher than 100 % and a specific surface area of 344.27 m2•g−1. The resulting high-purity ZSM-5 zeolite not only has high SiO2/Al2O3 molar ratio, good specific surface area, and regular hexagonal prism structure, but also has high crystallinity, smooth crystal surface and great grain homogeneity because of the microwave process. Its static adsorption capacities toward p-xylene and butyl acetate were 106.84 and 115.47 mg•g−1,

respectively, and the dynamic adsorption capacities were 81.44 and 176.14 mg•g−1, respectively. The preparation method of ZSM-5 zeolite with high efficiency and low cost proposed in this paper not only contributes to the high-value utilization of CGCS, but also provides an effective method and practical guidance for the removal of volatile organic compounds (VOCs).

- **Keywords:** ZSM-5 zeolite; Desilication solution; Microwave synthesis; Volatile organic compounds; Adsorption

Meriç Yılmaz Salman, Ergin Taşkan, Halil Hasar. *Comparative potentials of H2- and O2-MBfRs in removing multiple tetracycline antibiotics*. Pages 184-191.

Tetracycline antibiotics are broad spectrum antimicrobial compounds commonly used in human therapy and animal growth. This study has focused on the simultaneous removal of three tetracycline group antibiotics in co-existence in aquatic environments, including tetracycline (TC), oxytetracycline (OTC), chlortetracycline (CTC), and nitrous compounds in hydrogen (H2) and oxygen (O2) based membrane biofilm reactors (MBfRs). The treatment performances of MBfRs were comprehensively investigated by considering the effect of the hydraulic retention time (HRT) and surface loadings of tetracycline mixture. The results demonstrated that the average nitrification and denitrification efficiencies were 96% and 98% in H2-MBfR and O2-MBfR, respectively. The highest removal efficiencies for TC, OTC, and CTC in O2-MBfR were 52.5%, 54.83%, and 70.67%, while they were 92.5%, 90.5%, and 99.25% in H2-MBfR, respectively. The microbial analysis results showed that the dominant bacterial species in the biofilm of O2 and H2-based MBfRs belonged to the phyla Bacteroidetes and Proteobacteria. The findings of this study suggest that the MBfR process is an efficient alternative to remove tetracycline mixture and simultaneous nitrogen removal.

- **Keywords:** Membrane biofilm reactor; Tetracycline antibiotics; Antibiotic removal; Nitrification-denitrification; Microbial community

Xinrui Yuan, Kangping Cui, Yihan Chen, Shiyang Wu, Xinglong Liu, Haidong Diao. *Deciphering the response of biological nitrogen removal to gadolinium and sulfamethoxazole combined pollution: Performance, microbial community, and antibiotic resistance genes*. Pages 192-202.

Magnetic resonance imaging detection and the clinical treatment of bacterial infections in hospitals cause gadolinium and antibiotics to enter wastewater treatment plants (WWTPs). However, there remains missing information regarding the combined pollution of gadolinium and antibiotics in WWTPs. In this study, 50 μg/L of gadolinium (Gd(III)) and 500 μg/L of sulfamethoxazole (SMX) are selected to study their effects on the biological nitrogen removal performance, the microbial community structure, antibiotic resistance genes (ARGs), and mobile genetic elements (MGEs). The results demonstrated that Gd(III) and SMX combined pollution had an evident effect on denitrification, and elevated the abundance of ARGs by the increasing the abundance of intI1 in the MGEs. Moreover, Gd(III) inhibited the denitrification and decreased the abundance of ARGs. The distance heatmap showed that the typical nitrogen removal genes had a negative correlation with ARGs. This study highlights the effects of Gd(III) and SMX, both alone and coexisting, on nitrogen removal mechanisms, as well as the fate of ARGs and MGEs.

- **Keywords:** Combined pollution; Nitrogen removal; Microbial community; Antibiotic resistance genes; Mobile genetic elements

Guo-chang Song, Wen-ting Xu, Xing-yu Yang, Qiang Song. *Retention of As during coal combustion: Devolatilization and char combustion*. Pages 203-212.

The retention of arsenic (As) during coal combustion facilitates As emission control. A fixed-bed experimental system was used to conduct devolatilization and char combustion experiments at 1100–1300 °C using three types of coal. Both processes contributed to the As release. As in coal was bound to carbonate, oxide, sulfide, and aluminosilicate (Als-As). During devolatilization, carbonate- and oxide-bound As and Als-As remained stable, while sulfide-bound As was completely decomposed. The gaseous As was partially retained as Char-As. During char combustion, Char-As was oxidized to As2O3, which was partially retained by minerals. Carbonate- and oxide-bound As reacted with silicon (Si) and aluminum (Al) to produce Als-As, which was the main As form in ash. As retention was significantly inhibited by the destruction of the lattice structure. As retention by char during devolatilization and minerals during char combustion promoted As enrichment in solid products and its removal.

- **Keywords:** Arsenic; Retention; Coal; Devolatilization; Char combustion

Fabrice Ndayisenga, Zhisheng Yu, Bobo Wang, Gang Wu, Hongxun Zhang, Irfan Ali Phulpoto, Jie Zhao, Jie Yang. *Thermophilic-operating environment promotes hydrogen-producing microbial growth in a lignocellulose-fed DF-MEC system for enhanced biohydrogen evolution*. Pages 213-224.

This current work investigated the effects of increasing temperature on microbial biofilm composition during the conversion of the lignocellulosic agricultural wastes into biohydrogen using a dark-fermentation and Microbial electrolysis cell integrated system bio-catalyzed by a mixed culture. The reactors were operated under a thermophilic environment (R-Th) and directly compared with the reactors operated under mesophilic conditions (R-Me). The R-Th anodic biofilm composition was dominated by thermophilic lignocellulose-degrading and hydrogen-producing microorganisms belonging to the phyla of Proteobacteria (37.82 %), Thermotogota (35.94 %), and Coprothermobacteria (8.3 %) whereas the same phyla were noticeably less represented under mesophilic conditions. Compared to R-Th, R-Me anodic biofilm was characterized by more diverse microbial communities, and concomitantly promoted the proliferation of the methanogenic archaeal genera including Methanosarcina sp. (71.87 %), Methanothermobacter sp. (17.23 %), Methanomethylovorans sp. (8.35 %), Methanobrevibacter sp. (0.97 %), Methanobacterium sp. (0.79 %), Methanosphaera sp. (0.28 %), and Methanosaeta sp. (0.28 %). These results clearly show that the agricultural waste-fed DF-MEC integrated reactors performed under a thermophilic environment significantly promoted thermophilic-hydrogen producing microbial communities and inhibited the hydrogen-consuming microbial growth, which thus enhanced hydrogen yield. This work will significantly help the practitioners in selecting the suitable operating temperature during the fermentative conversion of agricultural wastes into biohydrogen energy on a large scale.

- **Keywords:** Hydrogen-producing bacteria; Fungal community; Methanogenic archaea; Agricultural wastes; Mesophilic and thermophilic environment; Dark fermentation and microbial electrolysis cell

Hong Lin, Lei Yang, Haochen Luan, Chang Han, Pingping Han, Hao Xu, Guoming Chen. *A data-driven assessment model for collision responses of offshore platform structure with ship using hybrid intelligent approaches*. Pages 225-246.

The accidents of ship collision with offshore platform bring huge risks to the safety of jacket structure. This paper proposed a data-driven assessment model for collision responses of offshore platform structure by integrating several intelligent and data-driven approaches. In the model, artificial neural network combining with dynamic particle swarm optimization algorithm (DPSO-ANN) is addressed to predict the collision responses of offshore platform structure, in which the uniform design method (UDM) is adopted to select training data. Principal component analysis (PCA) is used to eliminate correlation and redundancy of multivariate data of collision responses. Further, based on grey relational analysis (GRA), a GRA-based assessment index is established for the collision responses. In the case study, the prediction results demonstrate that the DPSO-ANN model could approximate the FEA (Finite Element Analysis) well, and the results of GRA-based assessment indicate that the collision velocity and mass of ship are two key factors influencing the collision responses of offshore structure. Also, the assessment results show that it is necessary to pay more attention and vigilance to the situations of high-speed approaching of large tonnage ship and ship berthing at low water level. The proposed model could serve as a beneficial and efficient assessment tool to support safety design of offshore platform structure under collision accidents.

- **Keywords:** Offshore platform structure; Assessment model; Uniform design method; DPSO-ANN; Principal component analysis; Grey relational analysis

Miao Jiang, Kun Wang, Ruiyuan Xue, Qingliang Zhao, Long Wang, Weiye Wang, Jing Ding. *Remediation of antimony-contaminated soil with composite materials of Fe/Fe2+-fly ash-concrete additive in seasonal freezing regions*. Pages 247-256.

Antimony (Sb) finds its wide application in industries, however, the research on Sb solidification/stabilization (S/S) in the Sb-contaminated soil is currently insufficient, particularly in seasonal freezing regions. Here six composite materials of Fe/Fe2+-fly ash-concrete additive (Fe-FA-CA) were employed and optimized to remediate the Sb-contaminated soil subject to 40 freezing-thawing (F-T) cycles. After remediation, FeSO4-fly ash-calcium lignosulfonate (FFC) exhibited the best resistance performance to F-T. The stabilization efficiency was evaluated with TCLP at 92.92%. Meanwhile, Sb concentration met the criteria of landfill for inert waste assessed with the compliance test for leaching (CT) of European Standard. The S/S efficiency of Sb dropped slightly from 92.68% to 88.22% (TCLP) and from 97.18% to 93.37% (CT), respectively, after aging 40 F-T cycles. The fraction of residual Sb in the soil treated by FFC was increased by 10.41%, and the strength of the S/S soil was much higher than 350 kPa, the requirement of landfills in the U.S. during F-T cycles. Additionally, the poorly crystalline Fe in the soil remediated by FFC was increased by 4.54 g/kg, suppressing Sb migration. The feasibility and effectiveness of FFC in S/S of Sb demonstrated its potential to remediate Sb-contaminated soil in seasonal freezing regions.

- **Keywords:** Antimony-contaminated soil; Solidification/stabilization; Fe/Fe2+-fly ash-concrete additive; Freezing-thawing cycles; Leaching concentration; Unconfined compressive strength

M. Tariq Nazir, A. Khalid, C. Wang, S. Akram, Y. Li, K.L. Wong, G.H. Yeoh. *Fire and electrically resistive silicone elastomer/alumina trihydrate composites derived from nanoclay and chopped glass fibres for industrial fire safety*. Pages 257-261.

Limiting oxygen index (LOI), flammability and electrical resistance of silicone elastomer (SiR)/alumina trihydrate (ATH) were investigated with the introduction of montmorillonite (MMT) nanoclay and chopped glass fibres (CGF). Results exhibited that MMT and/or CGF helped in improving the LOI and flame-retardant ability of SiR/ATH30. LOI of SiR/ATH30

was measured at 30% whilst it improved to 31% and 34% in MMT and/or CGF-filled composites. Interestingly, CGF offered better fire resistance to SiR/ATH30 than MMT. Moreover, the joint addition of MMT and CGF in the SiR/ATH30 exhibited the most improved flammability resistance. MMT/CGF slightly reduced the volume resistivity of SiR/ATH30 whereas, it is still measured as higher relative pristine SiR. Among all, SiR/ATH30/MMT5/CGF3 appeared a most promising candidate relatively with the peak heat release rate (pHRR), peak rate of smoke release (pRSR), peak mass loss rate (pMLR) and volume resistivity of 144.6 kW/m2, 1.53 (m2/s)/m2, 0.0436 g/s and 5.6 × 1010 Ω•cm.

- **Keywords:** Silicone rubber; Flame retardancy; Volume resistivity; Alumina trihydrate (ATH); Montmorillonite (MMT) nanoclay; Chopped glass fibre (CGF)

Gaofeng Zhu, Shuhua Xiong, Chen Shi, Yang Jin, Mingqiao Ge. *Activation of peroxydisulfate by Ce-doped Cu-Fe@γ-Al2O3 microspheres for polyvinyl alcohol, Reactive Red X-3B, and Rhodamine-B degradation*. Pages 262-273.

Advanced oxidation processes based on copper-iron bimetallic activated peroxydisulfate (PDS) can degrade pollutants, but the catalytic activation of PDS by copper-iron bimetallic catalysts can be further improved. In this work, Ce-doped Cu-Fe@γ-Al2O3 microspheres were fabricated and used to degrade polyvinyl alcohol (PVA). Contrast experiments showed that the Ce-doped Cu-Fe@γ-Al2O3/PDS system degraded 100 % of PVA after 180 s treatment at pH 7, a Ce(NO3)4·6H2O dosage of 15 %, a catalyst dosage of 1.25 g/L, a reaction temperature of 60 °C, and a PDS dosage of 2 g/L. Experiments showed that adding Ce atoms enhanced the stability and reusability of the catalyst containing copper and iron. In addition, the Cu-Fe@γ-Al2O3/PDS system showed degraded 99.98 % of Rhodamine-B and 99.96 % of Reactive Red X-3B dyes. EPR results showed that SO4·-, ·OH, O2·-, and 1O2 radicals were responsible for the degradation of PVA, Reactive Red X-3B, and Rhodamine-B. This study clarified the interaction mechanism between Ce, Cu, and Fe in the Cu-Fe@γ-Al2O3/PDS system. Our study provides guidance for improving the activation efficiency of PDS by Cu-Fe catalysts.

- **Keywords:** Polyvinyl alcohol; Peroxydisulfate; Catalyst; Degradation; Dyes

Feng Li, Xiaoxuan He, Yue Zhang, Chenchen Wang, Jia Tang, Runchuan Sun. *Superposition risk assessment of the working position of gas explosions in chinese coal mines*. Pages 274-283.

The prevention of gas explosion accidents is a key factor in enhancing the safety of production of coal mines. The effective management and control of the working position risks is of great significance for the prevention of such accidents. By analyzing data from 201 typical gas explosion accidents, 21 working positions related to the accidents were identified along with the main causing factors. By employing data statistical methods, the structural importance analysis method of fault tree analysis, and the summation method, the risk associated with each working position was evaluated. Then, this work built a risk assessment matrix to categorize risk levels associated with various working positions related to gas explosions in coal mines. Also, based on the kernel density analysis, a superposition risk assessment model was established. In addition, the ArcGIS software was used to simulate and calculate the superimposed risks and draw a risk distribution map. The results show that the number of working positions of Level I is mainly affecting the fully mechanized mining team, the fully mechanized excavation team, and the ventilation team. The risk distribution map intuitively shows that the high-risk working positions involving gas explosion accidents in Chinese coal mines mainly exist in the working face and the tunneling face. It is highlighted that the working position risk and grade distribution have a significant hierarchy after risk superposition.

- **Keywords:** Coal mine gas explosions; Working position risk; Superposition risk; Kernel density analysis; Risk classification

By Jianguo Liu, Shu Wang, Longzhe Jin, Yixuan Wei, Shengnan Ou, Tianyang Wang, Jingge Xu, Xianfeng Liu, Guoyin Tao. *Surface pore characteristics of original coal dust produced in underground mining sites and their impact on the moisture content*. Pages 284-298.

In underground coal mines, the efficiency of water-based dust suppression technologies is heavily limited by the poor wettability of coal dust. To explore the effect reasons of the surface pore parameters of coal dust on its wettability, in this study, 18 original coal dust (OCD) samples produced in underground mining sites were collected from various underground coal mines in north China. The surface micropore (pore size <2 nm) and mesopore (2 nm < pore size <50 nm) characteristics of the OCD samples were measured with the nitrogen (N2) adsorption/desorption method. Subsequently, the correlations between the pore characteristics of the OCD samples and their moisture contents and initial contact angle (ICA) were established and discussed. The results demonstrate that the pore structures of the OCD samples are significantly developed, and the impermeable pores with one open end are the dominant pore types in the OCD. The micropore structure of the OCD samples considerably affects its moisture content, thus influencing its wettability. As the increase of micropore size, micropore volume, and specific surface area (SSA), the moisture content of the OCD samples linearly decreased (R2 =0.55), linearly increased (R2 =0.66), and linearly increased (R2 =0.65), respectively. The large capillary force caused by the developed SSA accounts for the significant moisture conservation property of the micropore structures, which improves the wettability of the OCD. The variation of the ICA with the pore parameters well verifies this conclusion.

- **Keywords:** Coal dust; Dust suppression; Pore characteristics; Fractal dimensions; Moisture content

Huanli Sun, Lin Zhang, Qiangling Duan, Shuyang Wang, Shijie Sun, Jinhua Sun, Qingsong Wang. *Experimental study on suppressing thermal runaway propagation of lithium-ion batteries in confined space by various fire extinguishing agents*. P.ages 299-307.

Thermal runaway initiated in an individual cell may transfer heat to adjacent cells, and cause thermal runaway propagation. Thus, mitigation and prevention of thermal runaway propagation using extinguishing agents are significant. In this work, fire and extinguishing tests on 117 Ah LIBs with Li(Ni0.8Co0.1Mn0.1)O2 (NCM)/graphite electrodes are investigated. The suppression effects of different extinguishing agents including HFC-227ea, C6F12O and water spray on thermal runaway propagation in confined space were compared. Results show that thermal runaway propagation can occur in LIBs module even with thermal management measures. When activated immediately after the thermal runaway of the first cell, each agent can extinguish the LIBs module fire. However, the cooling capacity of extinguishing agent is the key factor to suppress thermal runaway propagation. The heat dissipation of HFC-227ea, C6F12O and water spray in fire extinguishing test is 24.8 kJ, 111 kJ and 459.8 kJ, respectively. Thus, HFC-227ea can hardly suppress the thermal runaway propagation. Although C6F12O can not prevent thermal runaway propagation, it can decrease the battery temperature, slow down the heat transfer rate and prolong the propagation time. While water spray has the best cooling effect, which can prevent thermal runaway propagation.

- **Keywords:** Lithium-ion battery safety; Thermal runaway propagation; Fire extinguishing agents; Suppressing effectiveness

Ziyu Zou, Ercheng Zhao, Pingzhong Yu, Junjie Jing, Ying Li, Baotong Li, Junxue Wu. *Simultaneous remediation of three neonicotinoids in soil using nanoscale zero-valent iron-activated persulfate process: Performance, effect of process parameters, and mechanisms*. Pages 308-321.

Neonicotinoids are commonly used pesticides in agricultural regions all over the world, and their widespread use has caused potential environmental pollution issues in recent years. The simultaneous degradation of three representative neonicotinoids (i.e., imidacloprid (IMI), thiamethoxam (TMX) and dinotefuran (DIN)) in soil by a nanoscale zero-valent iron-activated persulfate (nZVI-activated PS) process was investigated. Under the optimum conditions with 1 mg g−1 nZVI, 10 mM PS at an initial pH value of 6.9 and a water-soil ratio of 1.5, the degradation efficiency of IMI, TMX and DIN reached 89%, 86% and 69% in 15 mins, respectively. Degradation of the three neonicotinoids was fitted with a pseudo first-order kinetic model. High nZVI dosage and PS concentration were found to enhance the neonicotinoids degradation. In contrast, the presence of Cl-, HCO3- and HA reduced the degradation rates of the three neonicotinoids. Soil physicochemical properties showed a significant effect on the degradation efficiencies of the three neonicotinoids. In addition, quenching experiments combined with electron paramagnetic resonance (EPR) showed that free radicals SO4•- and •OH contributed to the degradation of three neonicotinoids in the nZVI-activated PS system. Degradation pathways were proposed based on identified intermediates of IMI, TMX and DIN. Overall, the nZVI-activated PS process is an effective method for remediation of the neonicotinoids contaminated soil.

- **Keywords:** Neonicotinoids; Degradation; Soil remediation; Nanoscale zero-valent iron; Persulfate

Yang Zhang, Bingding Shi, Baozhong Ma, Zhihe Cao, Shuang Shao, Yubo Liu, Xiang Li, Chengyan Wang, Weijiao Yang. *Removal of fluoride from waste acid using lanthanum chloride: Defluoridation behavior and reaction kinetics of recovery process*. Pages 322-331.

Waste acid would bring serious fluoride pollution. In this study, a fluoride removal method for waste acid using lanthanum chloride (LaCl3) was proposed. This process consists of three parts, removal of fluoride, collection of lanthanum, and transformation of lanthanum fluoride (LaF3). The E-pH diagram of the La-F-H2O system was constructed to learn about the composition variation of the system with pH. The removal efficiency of fluoride was 98.03%, and F− was reduced to 20 mg/L under the optimal conditions of the n(LaCl3):n(F−) of 1:1, the temperature of 80 °C, and the reaction time of 8 h. The residual lanthanum in the solution was collected as sodium lanthanum sulfate (NaLa(SO4)2) precipitate by sodium sulfate (Na2SO4), and the collection efficiency of lanthanum was 98.05%. The defluoridation product LaF3 was transformed to lanthanum hydroxide (La(OH)3) by sodium hydroxide (NaOH) solution, and the transformation efficiency was 93.44%. The adsorption phenomenon of La(OH)3 to F− was found in the transformation process, which is not conducive to the recovery of La. The kinetics of the transformation process of LaF3 to La(OH)3 shows that the rate-controlling step is the diffusion of the solid product layer, and the average apparent activation energy is 37.99 kJ/mol at 25–100 °C.

- **Keywords:** Waste acid; Fluoride removal; Rare earth; Defluoridation behavior; Reaction kinetics

Akshit Trada, Amita Chaudhary, Dhruvil Patel, Darshit S. Upadhyay. *An alternative fuel production from sawdust through batch-type pyrolysis reactor: Fuel properties and thermodynamic analysis*. Pages 332-342.

This paper deals with the experimental investigations and thermodynamic studies carried out for five distinct temperatures ranging from 300 to 500 ℃ with a heating rate of 10 ℃/min. This work aims to study the influence of pyrolysis temperature on product (biochar, bio-oil, syngas) yield, its physicochemical properties and energy yield. The experiments were conducted in a batch-type vacuum pyrolysis reactor with sawdust as a feedstock. Findings show that biochar yield declined with temperature rise, whereas bio-oil and syngas yield increased. A higher yield of bio-oil (40.67%) was obtained at 450 ℃; after that it was declined. However, a higher biochar yield (60.67%) was attained at 300 ℃. Syngas generated at 500 ℃ had a higher product yield (24%) and energy output (147.05 kJ). Although, total energy output was found to be higher at 500 ℃ (634.71 kJ). This research also included thermodynamic studies such as mass, energy, exergy analysis, and sustainability analysis and found good agreement between input and output parameters. The study's main conclusion is that higher pyrolysis temperatures (450–500 ℃) offer better results in terms of higher product and energy yield for sawdust feedstock.

- **Keywords:** Pyrolysis; Sawdust; Biochar; Pyro-oil; Syngas; Thermodynamic analysis

Lingqiang Yan, Jinlong Li, Xue Jian, Xinhao Li, Jianyu Zhang, Qing Ye. Evaluation on the separation effect and extractant recovery efficiency of extractive distillation for separating ethyl acetate/methanol with ionic liquids as extractants. Pages 343-355.

For the purpose of recycling resource and cleaner production, the extractive distillation schemes with different ionic liquids as extractants are proposed to separate ethyl acetate and methanol. In fact, the evaluation of extractants should not just focus on the separation effect, the effectiveness for the recovery of extractants which has a great influence on the overall benefits of extractive distillation process also need to be paid more attention, especially for the ionic liquids (ILs). On the basis of the VLE diagram, σ-Profiles, and interaction energy based on molecular dynamics, the separation effects of the selected extractant are following the order of 1-ethyl-3-methylimidazolium acetate ([EMIM][OAc]) > 1-ethyl-3-methylimidazolium diethyl phosphate ([EMIM][DEP]) > dimethyl sulfoxide (DMSO). However, the decomposition temperature of [EMIM][DEP] is much higher than that of [EMIM][OAc], which leads to the better effectiveness for extractant recovery. Then, several recovery configurations are explored owing to different decomposition temperature of selected ILs. The result shows that the heat integration assisted the process with [EMIM][DEP] as extractant which utilizes two-stage evaporators extractant recovery configuration has a better performance than other processes and can reduce 35.07% of TAC, 37.59% of energy consumption and 37.36% of gas emission compared with conventional extractive distillation process with DMSO as extractant

- **Keywords:** Ionic liquids; Separation effect; Decomposition temperature; Extractant recovery

Jiaxing Zhu, Zixuan Liu, Zhengrong Cao, Xiaoyi Han, Lin Hao, Hongyuan Wei. *Development of a general inherent safety assessment tool at early design stage of chemical process*. Pages 356-367.

The purpose of process safety is the prevention and mitigation of incidents arising from process-related hazards while inherent safety design is one of the most effective ways to prevent accidents in the process safety management. Inherent safety assessment tools (ISATs) play an important role in the application of inherent safety design. However, many ISATs suffer from various limitations. Hence, we propose a general inherent safety assessment tool to evaluate inherent safety level at the early design stage of chemical

process. First, we define two criteria of good inherent safety assessment tools from their purpose, namely reliability and usability. We link the inherent consequence to process parameter and chemical property, subsequently propose a general inherent safety assessment tool for different hazardous sources (e.g., and fire/ explosion, health, environment). The proposed tool can eliminate the uncertainties in the risk-based inherent safety assessment tools and address the problem that the amount of material handled is not considered in the continuous numerical assessment tools. Finally, we use two cases to illustrate the proposed inherent safety assessment tool and compare with the commonly used ISATs. This work can accelerate the inherent safety design at the early design stage to prevent incidents in the chemical process.

- **Keywords:** Process safety; Inherent safety design; Inherent safety assessment tool; Quantitative risk analysis; Chemical process

Heejin Yang, Jin-Kyu Kang, Sanghyun Jeong, Seong-Jik Park, Chang-Gu Lee. *Removal of perfluorooctanoic acid from water using peroxydisulfate/layered double hydroxide system: Optimization using response surface methodology and artificial neural network*. Pages 368-377.

As perfluorooctanoic acid (PFOA) cannot be effectively removed using existing water treatment methods, research on PFOA removal is attracting increasing attention. In this study, PFOA removal was examined using layered double hydroxide (LDH) as an adsorbent as well as a heterogeneous catalyst for peroxydisulfate (PDS) activation. Based on the central composite design (CCD) experiment results, the optimal conditions for PFOA removal were a PDS concentration of 5 mM, LDH dose of 1 g/L, and initial pH of 2.5. The predictability of PFOA removal using response surface methodology (RSM) and an artificial neural network (ANN) showed significant differences between RSM and ANN in non-CCD conditions, with higher predictability (R-value = 0.7574) in RSM. A scavenger test was performed to analyze the effect of radicals generated during PDS activation, and the PFOA removal rate increased from 64 % to 83 % by controlling the hydroxyl radical using a chemical scavenger, which was verified through electron spin resonance analysis. Additionally, the prepared LDH showed high stability based on the reuse experiments and characterization results. These results suggest that the PDS/LDH system can be an attractive solution for the removal of PFOA by adsorption and degradation in wastewater and can optimize operational processes through multi-parameter modeling.

- **Keywords:** Perfluorooctanoic acid; Peroxydisulfate; Layered double hydroxide; Multi-parameter modeling; Hydroxyl radical restraint

Yikang Tu, Zijian Su, Yingxian Zhu, Yuanbo Zhang, Juan Xu, Tao Jiang. *A detoxification and value-added process for chromium ore processing residue (COPR) and Fe-C-bearing dust: Direct reduction-magnetic separation*. Pages 378-389.

Chromium ore processing residue (COPR), containing much virulent hexavalent chromium [Cr(VI)], is a by-product derived from chromate production. Fe-C-bearing dust from steel industry is very difficult to be utilized effectively because of its complex composition and unstable properties. The dust was co-processed with COPR by a direct reduction-magnetic separation process in this study. Through the strong reducing ability of solid carbon in Fe-C-bearing dust, the compounds of Cr and Fe were reduced to (Cr, Fe)7C3 alloy during the reduction roasting process and then selectively recovered by magnetic separation. In addition, the Pb and Zn compounds were reduced and volatilized into flue gas at high temperature. Under the optimal conditions, the results indicated that Cr-containing iron powder with 72.59 % Fe and 6.34 % Cr was obtained, and the recoveries of Fe and Cr were respectively 79.1 % and 76.9 %. The volatilization rates of

Pb and Zn met 97.47 % and 99.95 %, respectively. The non-magnetic tailings were determined to be nontoxic and could be used as high-quality raw materials for building.

- **Keywords:** COPR; Fe-C-bearing dust; Detoxification; Selective recovery

Dong Chen, Yan Kuang, Haoyu Wang, Jingjing Liang, Jianwei Zhao. *Insights into the mechanism of naproxen inhibiting biohydrogen production from sludge dark fermentation*. Pages 390-397.

In order to explore the effect of emerging pollutant naproxen (NPX) on the hydrogen production from excess sludge(ES) dark fermentation, six groups of laboratory-scale sequencing batch anaerobic reactor were constructed. The biohydrogen production efficiency, the transformation characteristics of organic matter and the activities of key enzymes were analyzed to explore the effect of NPX on the ES dark fermentation hydrogen production. The effect of NPX on ES dark fermentation is closely related to its exposure content, that is, low-dose NPX had no obvious effect on biohydrogen production, while high-dose NPX inhibited biohydrogen production. 12.0 mg NPX/Kg reduced biohydrogen production to 14.6 mL/g, about 12.5 % of the control. NPX can be partially removed in the process of ES dark fermentation, and the removal efficiency was about 23.3~42.5 %. NPX promoted the release of dissolved chemical oxygen demand (COD) and increased the soluble organic matter in the fermentation broth. However, NPX significantly suppressed the acidification process, which was also the key reason for the decline of biohydrogen production. Enzyme activity analysis also verified the inhibition of NPX on key enzymes involved in volatile fatty acids (VFA) and biohydrogen production. The results of this study enriched the influence behavior of NPX in the environment, and provided a certain theoretical basis for the ES resource utilization.

- **Keywords:** Naproxen; Excess sludge; Dark fermentation; Biohydrogen production; Enzymatic activity

Milad Rajaei, Sara Nazif. *Improving wastewater treatment plant performance based on effluent quality, operational costs, and reliability using control strategies for water and sludge lines*. Pages 398-411.

As a result of urbanization and population growth, wastewater treatment plants (WWTPs) are experiencing increased influent flow rates, pollutant loads, and stricter standards for effluent quality. Therefore, implementing a control strategy is critical for improving the performance of WWTPs in response to highly variable effluent quality. In this study, different strategies for both water and sludge lines are deployed in WWTP model to control dissolved oxygen and biomass concentration in activated sludge system by manipulating aeration intensity and sludge flow rates. The efficiency of suggested control strategies is evaluated using different performance criteria, including effluent quality indicators, operational costs, and system reliability. The proposed method is applied in a real WWTP located in south of Tehran, the capital of Iran. According to the findings, controlling aeration system and sludge flow rate improve effluent quality and system reliability despite increasing operational costs. In the case of simultaneous control of water and sludge lines, the effluent quality index has improved by 9.3%, while the operational costs have increased by 1%. Moreover, the system reliability based on effluent ammonia, TSS, and COD concentration have increased by 33.4%, 9%, and 12.2%, respectively.

- **Keywords:** Wastewater treatment plant modeling; Control strategy; Reliability

Xinhong Li, Yazhou Liu, Rouzbeh Abbassi, Faisal Khan, Renren Zhang. *A Copula-Bayesian approach for risk assessment of decommissioning operation of aging subsea pipelines*. Pages 412-422.

Currently, many subsea pipelines are reaching their design life, and most of them need to be decommissioned due to the serious structural degradation. However, the decommissioning operation of aging subsea pipelines is a challenging task due to the harsh environmental and technical complexity. An efficient risk assessment is important to ensure the safety of pipeline decommissioning operation. This paper presents a Copula-Bayesian approach for risk assessment of decommissioning operation of subsea pipelines, which can capture the complicated interactions among risk factors of decommissioning operation of subsea pipelines. The correlations among risk factors are described qualitatively and quantitatively using the percentile cobweb plot and correlation coefficients. The critical risk factors in decommissioning operation can be found by correlation analysis. Finally, the failure probabilities of pipeline decommissioning operation are estimated. The methodology is tested by a case study of decommissioning operation of a subsea pipeline in the South China Sea. The results indicate that the improper cutting technique, operation error, and unqualified construction are the critical risk factors, and the failure probability of decommissioning operation is positively correlated with the update on the critical risk factors. The methodology can be a useful tool for risk-informed decision-making in subsea pipeline decommissioning operation.

- **Keywords:** Aging subsea pipelines; Decommissioning operation; Copula-Bayesian approach; Risk assessment

Youqi Tao, Rui Shi, Liurui Peng, Maoyuan Yang, Yuecheng He, Qian Huang, Wenlai Xu. *Start-up characteristics and microbial nitrogen removal mechanisms in ANAMMOX systems with different inoculations under prolonged starvation*. Pages 423-433.

The characteristics of lab-scale ANAMMOX system for efficient nitrogen removal were tested by different inoculations (anaerobic granular sludge (AGS) + anammox sludge (AMS), R1; AGS alone, R2) in continuous flow reactors following start-up under starvation. TN removal rates were above 90 % in both reactors. Microbial community analysis showed that the nitrogen removal was the combined results of anammox and partial denitrification (PD), Higher microbial growth rate triggered by quorum-sensing (QS) caused R1 to secrete more extracellular polymeric substances (EPS) and promoted the growth of its particle size. However, the overproduction of EPS destroyed the particle structure with time, and led to a deterioration of operational stability in R1. R2 showed better nitrogen removal stability to high nitrogen loading rate (NLR). This was due to higher endogenous organics within R2, which inhibited cell aggregation and EPS overproduction. But undeniably, R1 had higher specific anammox activity (SAA) with higher anammox bacteria (AAOB) abundance (The abundance of Planctomycetota in R1 and R2 were 21.2 %, 7.71 %). The results suggest that the operational stability was influenced by a combination of particle properties and microbial metabolism, and that the inoculation of AGS is more conducive to efficient and economic nitrogen removal in wastewater treatment under starvation.

- **Keywords:** Anammox; Particle characteristics; Starvation shock; Start-up; Multiple bacterial communities

Naisini Ariram, Srinivasan Pradeep, Sundarapandiyan Sundaramoorthy, Balaraman Madhan. *Single pot low float chromium tanning: Cleaner pathway approach to environment friendly leather manufacturing*. Pages 434-442.

Chromium tanning is the most essential and extensively used tanning process in leather manufacture that requires pre and post-treatment steps such as pickling and basification to stabilize the collagen in the skin matrix. The conventional chromium tanning process results in low chromium uptake. The unabsorbed chemicals end up in the effluent,

directly affecting the environment. Stringent norms have been stipulated for the disposal of effluents containing chromium, total dissolved solids and chlorides, forcing tanners to explore low-waste and cleaner chromium tanning processes. A chemical mixture was formulated to overcome the issues associated with chromium tanning process, which leads to pickle and basification free single pot chromium tanning. The designed process reduces effluent load generation exhibiting nearly 99% chromium uptake, while the conventional chromium uptake is only about 69%. The experimental process results in more than 99% reduction in TDS, chlorides, and COD load compared to the conventional tanning process. Also, the experimental leather possesses good thermal stability and physical strength comparable to the conventional leathers. Thus, the present research work provides an option for cleaner tanning technology to reduce water and chemical load, and the system is environmentally friendly.

- **Keywords:** Low-float chromium tanning; Pickle free; Basification free; Cleaner tanning technology

Xi Chao, Ting-an Zhang, Guozhi Lv, Aichun Zhao, Zhipeng Liang, Shengnan Lin, Yang Chen, Qiuyue Zhao, Fangqin Cheng. *A novel process for one-step preparing potassium-containing fertilizer using red mud or CFA synergistic extraction of alumina*. Pages 443-453.

Red mud and coal fly ash (CFA) are bulk aluminum-containing solid waste in the industrial production process, posing a great threat to the environment and ecological security. The present paper proposes a novel method for one-step producing potassium-containing fertilizer synergistically extracting Al2O3 by KOH hydrothermally treating red mud or CFA. In this paper, the dissolving ratio of Al2O3 in the K2O-Al2O3-H2O ternary system and the extraction of Al2O3 from red mud or CFA after hydrothermal treatment with KOH were investigated. The phase structure transformation of leaching residue obtained under various conditions was analyzed by X-ray diffraction and scanning electron microscopy, and the fertilization efficiency of the products was verified by potting experiments. The results show that the dissolving ratio of Al2O3 can reach the highest value of 85.04% at 120 °C with the K2O mass fraction of 24.90% in the ternary system. When red mud or CFA was hydrothermally leached with 240 g/L K2O at 240 ℃, the Al2O3 extraction rates of 25.50% and 31.42% could be separately obtained, and the leachate could be reused. The main phases of the leaching residue were kaliophilite, illite, and megakalsilite, and the content of K2O was 7.83% and 26.89%, which can be applied as potassium-containing fertilizer to improve soil fertility and effectively promote the growth of pakchoi. The process improves the comprehensive utilization of red mud and CFA without secondary pollution, reduces the negative impact on the environment, and opens up a new way to apply bulk solid waste in the agricultural field.

- **Keywords:** Red mud; Coal fly ash; Hydrothermal leaching; Potassium-containing fertilizer

Nandini Bhambore, M. Suresh Kumar. *Municipal solid waste generation, management scenarios, and leachate treatment using sequencing batch biofilter granular reactor*. Pages 454-468.

Unsegregated MSW disposal in Landfills, generation of leachate, and its contamination is a worldwide problem. These highly toxic organic content in the leachates require proper disposal. Traditional treatment processes are not adequate enough to tackle the problem, and sludge generation in the treatment process is one of the major hurdles. For this, sequencing batch biofilter granular reactor (SBBGR) has been found to be an exceptional solution with greater flexibility, more compactness, and less sludge generation. In the present study, we review the mechanism and performance of SBBGR for leachate treatment and a comparison with available conventional wastewater treatment

processes. SBBGR mechanism is based on the granular biomass formation in the reactor with the feast and famine phenomena and retaining on support media provided in the microaerophilic zone of the reactor. SBBGR has been found to be highly efficient for removing COD, total nitrogen, TOC, TSS, etc. SBBGR has also been discussed for its excellent removal efficiency in the removal of emerging contaminants like microplastics and endocrine-disrupting chemicals. The present review highlights the advancements in the SBBGR-based process in recent decades that have been summarized. Finally, this review also indicates various factors affecting the performance of SBBGR along with its favored benefits.

- **Keywords:** Landfill leachate; Wastewater treatment processes; Feast and famine; Aerobic granulation; Biofilters

Wenhao Huang, Zhenshan Huang, Zhuoyao Chen, Zuotong Wu, Zaishan Wei. *Biostabilization of cadmium-containing flue gas by sulfate reducing membrane biofilm reactor*. Pages 469-479.

Flue gas cadmium may endanger human health and ecological environment due to its persistent, toxic and bioaccumulating. A sulfate reducing membrane biofilm reactor (MBfR) for removal of cadmium-containing flue gas was investigated. Cadmium removal efficiency was up to 95.1%. Desulfovibrio was the dominant genus. Desulfovibrio, Desulfomicrobium, Pseudodesulfovibrio were the core cadmium-resistance-sulfate-reducing genus. Cadmium resistance proteins (transcriptional regulatory protein, efflux protein, binding protein and heavy-metal associated domain protein) and sulfate-reducing enzymes (Sat, AprA, AprB, DsrA, DsrB) involved in the regulation of cadmium stress and dissimilar sulfate reduction. The biofilm was characterized by FTIR, XPS, XRD, EEM, and SEM-EDS. XPS and XRD spectra indicate the formation of a cadmium sulfide (CdS) from flue gas cadmium conversion. Humic acid complex arsenic (HA-Cd) and CdS coprecipitation were formed in MBfR system. Cadmium-containing flue gas was bio-stabilized in the form of CdS and HA-Cd via complexation of humic acids in extracellular polymeric substances (EPS), biosorption and biodeposition. These results show that the sulfate-reducing membrane biofilm reactor is achievable and open new possibilities for applying the MBfR to removal of cadmium-containing flue gas.

- **Keywords:** Cadmium in flue gas; Sulfate reducing bacteria; Biostabilization; Biosorption; Biodeposition

Zhenchao Wei, Xu Ji, Li Zhou, Yagu Dang, Yiyang Dai. *A novel deep learning model based on target transformer for fault diagnosis of chemical process*. Pages 480-492.

Deep learning is a powerful tool for feature representation, and many methods based on convolutional neural networks (CNNs) and recurrent neural networks (RNNs) have been applied on fault diagnoses for chemical processes. However, unlike attention mechanisms, these networks are inefficient when extracting features of long-term dependencies. The transformer method employs a self-attention mechanism and sequence-to-sequence model originally designed for natural language processing (NLP). This approach has attracted significant attention in recent years due to its great success in NLP fields. The fault diagnosis of a chemical process is a task based on multi-variable time series, which are similar to text sequences with a greater focus on long-term dependencies. This paper proposes a modified transformer model called Target Transformer, which includes not only a self-attention mechanism, but also a target-attention mechanism for chemical process fault diagnoses. The Tennessee Eastman (TE) process was used to evaluate our method's performance.

- **Keywords:** Fault diagnosis; Deep learning; Attention mechanism; Transformer

Jun Xie, Liansheng Liu, Xuanchen Liu, Huiru Qu, Runze Duan. *Effect of bubble cutting on spray characteristics and dust control performance in the effervescent atomization*. Pages 493-499.

Effervescent atomization performance depends on the bubble size inside the mixing chamber, consequently influencing the spray dust control performance. This paper proposes an optimization of atomization quality and dust control performance by incorporating a bubble cutter in the atomizer mixing chamber. The effects of the bubble cutter aperture on spray characteristics and flow characteristics were experimentally investigated under different operating conditions. Experimental results showed that Sauter means diameter (SMD) decreases with increasing injection pressure and gas-liquid mass flow ratio (GLR). Furthermore, SMD initially increased and then decreased by reducing the aperture of the bubble cutter from 500 μm to 80 μm. In particular, high injection pressure (Pi =0.6 MPa) and low gas-liquid mass flow ratio (GLR=0.09) strengthened the effects of the bubble cutter aperture on SMD. Moreover, bubble cutter causes a contiguous concentrated droplet size distribution, but it has little effect on droplet velocity. Ultimately, the optimal bubble cutter aperture on the efficiency of respirable dust control efficiencies was theoretically calculated. The dust control efficiency is a maximum at the bubble cutter with an aperture of 230 μm for the effervescent atomizer in this paper. Spray dust control efficiency reaches 93.15 %, which effectively solves the problem of high dust concentration pollution in the mechanized working environment.

- **Keywords:** Spray dust control; Effervescent atomizer; Spray characteristic; Droplets size distribution; Bubble cutter

João Pedro Bachega Cruz, Edilson Gabriel Veruz, Idalina Vieira Aoki, Adriana Miralles Schleder, Gilberto Francisco Martha de Souza, Gustavo Leitão Vaz, Leonardo Oliveira de Barros, Rene Thiago Capelari Orlowski, Marcelo Ramos Martins. *Uniform corrosion assessment in oil and gas pipelines using corrosion prediction models – Part 1: models performance and limitations for operational field cases*. Pages 500-515.

Internal and uniform corrosion caused by the presence of corrosive gases CO2 and/or H2S in the inner stream is the major inherent concern of the oil and gas industry regarding its carbon steel pipelines selected for the processes present in hydrocarbons production and transportation, which culminates in generalized loss of thickness along the pipelines surface. Distinct corrosion predictive models have been developed and updated for the prediction of this corrosive mechanism through main multiphase flow physical-chemical parameters, however, worries regarding models' uncertainties and limitations remains. This study reviews and compares the most common predictive models in the industry, clarifying its classifications and input parameters. Based on that, NORSOK, OLI and Predict models are applied to oil and gas operational field cases from literature and the implementation of a preliminary sensitivity analysis of models' parameters for these applications is done. The progress allowed the operational cases histories evaluation and the elucidation of the main constraints of corrosion data collection by industry and of predictive models application. Moreover, this study discusses preliminary perspectives about models' uncertainty and presents the pH as the most important influential parameter in uniform corrosion prediction, forwarding the necessary future development for corrosion assessment in operational pipelines.

- **Keywords:** Uniform corrosion assessment; Corrosion prediction models; Sensitivity analysis; Case histories evaluation; Oil and gas industry; Carbon steel pipelines

Javad Yahaghi, Alireza Bazargan. *The synergetic effects of radio-frequency electromagnetic field and pH adjustment on landfill leachate microbial inactivation*. Pages 516-526.

Landfill Leachate (LFL) treatment is a challenging and complex issue. One such difficulty is biofouling or bio-clogging caused by the rich microbiome of the LFL. In this study, the effect of Radio Frequency Electromagnetic Field (RFEMF) inductance on the microbial inactivation of LFL has been investigated for the first time, and it is shown that RFEMF alone can result in 24–35% reduction in LFL microbial count. Meanwhile, the application of the electromagnetic field alongside pH adjustment is shown to significantly reduce the bacterial count of the LFL, from over 9 × 104 CFU/mL to under 1.5 × 104 CFU/mL under optimum conditions. In other words, the application of RFEMF with pH adjustment shows very strong synergetic effects, increasing the effectiveness of the treatment more than two-fold. The reason for this observation is the damage caused to the cell membranes via pH adjustment, making the microorganisms particularly vulnerable to the effects of the RFEMF. This study offers a low-cost and simple method for disinfection, and highlights an avenue of research on microbial inactivation, not just for LFL but possibly for other wastewater streams as well.

- **Keywords:** Disinfection; Bacteria removal; Microbial count; Physical treatment; Municipal solid waste

Débora Federici dos Santos, Wardleison Martins Moreira, Thiago Peixoto de Araújo, Rosângela Bergamasco, Indianara Conceição Ostroski, Maria Angélica Simões Dornellas de Barros. *Non-conventional processes applied for the removal of pharmaceutics compounds in waters: A review*. Pages 527-542.

The increasing occurrence of pharmaceuticals in the ecosystem is considered a global concern. These substances easily reach water and wastewater treatment systems and water bodies through the industrial, hospital, and residential effluent discharges, human and animal urine and feces, fertilizers, and disposal of medicines in common garbage or sinks. These drugs, even at low concentrations, when present in the environment, can cause changes in the endocrine, immune, and reproductive systems of living things there. In this context, this article presented an overview of where drugs such as caffeine, paracetamol, and diclofenac were found worldwide. In addition, this review set out to discuss how these drugs affect the quality of the water and all the beings around it. Therefore, this review aims to provide a deeper and more critical systematic approach to non-conventional processes such as adsorption, advanced oxidative processes, and membranes that can be employed to remove caffeine, paracetamol, and/or diclofenac from water. To this end, theoretical concepts were expounded, and scientific articles published in the literature on these advanced treatments between 2010 and 2022 were analyzed. This review will be valuable for researchers studying advanced processes to remove emerging contaminants.

- **Keywords:** Pharmaceutical pollution; Emerging drugs; Detection; Water treatment; Removal processes

Michael L. Hobbs, Phillip F. Britt, David T. Hobbs, Michael J. Kaneshige, Michael Minette, Jessica Mintz, Frank M. Pennebaker, Gary R. Parker Jr., Robert Pierce, David M. Rosenberg, Jon Schwantes, Audrey Williams. *Thermal runaway of nitric acid-soaked kitty litter in transuranic waste*. Pages 543-549.

Precise wording is important in every field of study, including operational procedures. Confusion in the wording “organic” and “inorganic” may have contributed to substitution

of an organic kitty litter for an inorganic adsorbent used to prepare nuclear waste for disposal at an underground salt repository. Adsorbents prevent liquids like nitric acid from causing corrosion within the waste drums. However, combination of organic material with nitric acid can cause heat- and gas-generating reactions resulting in thermal runaway, rapid pressurization, and drum rupture. In 2014, waste Drum 68660 containing nitric acid-soaked organic kitty litter exploded and released transuranic waste into the repository. The cause of the accident was never identified. Here we show that the root cause of Drum 68660 igniting was restriction of the drum vent resulting in accelerated nitric acid chemistry, thermal runaway, and radiation dispersal.

- **Keywords:** Thermal hazard; Waste behavior; Waste characteristics; Safety analysis; Cookoff

Zanlang Tang, Haonan Liu, Zeyu Xiao, Xincun Tang. *A novel process of immobilizing sodium arsenate crystals as scorodite using Fe(OH)3 as an iron source*. Pages 550-564.

Sodium arsenate crystals are a hazardous waste produced from the utilization of arsenic–alkali residue in antimony metallurgy that pose a serious threat to the environment. In this article, to eradicate the damage caused by sodium arsenate and enhance the sustainable development of nonferrous metallurgy, a novel process was proposed to immobilize arsenic as flaky scorodite using Fe(OH)3 as an iron source. Various methods, such as X-ray diffraction (XRD), scanning electron microscopy (SEM), and inductively coupled plasma atomic emission spectrometry (ICPAES), were applied to characterize these synthesized products. The whole process is divided into three parts. In the thermodynamic analysis, the stable area of scorodite in the Pourbaix diagram significantly expands at high ionic activity and temperature, which favors the decrease in $\triangle rG$ for scorodite synthesis, and Fe–As coprecipitation is feasible in solution at $0.18 \leq pH \leq 5.30$. In the scorodite synthesis, 99.88% of the arsenic was converted to a flaky scorodite with a size of 2–5 μm by optimizing the parameters. In the removal of arsenic, residual arsenic and iron were completely coprecipitated into an iron salt by dropping NaOH solution to a final pH of 5.0. The final products include scorodite and sodium sulfate in this process. Overall, this new approach successfully eliminates the potential arsenic pollution from the utilization of arsenic–alkali residue in antimony metallurgy and can potentially be applied to dispose of other high arsenic-bearing wastes.

- **Keywords:** Sodium arsenate; Ferric hydroxide; Scorodite; Sodium sulfate

Tian Wang, Jia Xu. *Nonlinear analysis on the influence of rainfall: A new way to eliminate air pollution*. Pages 565-575.

In this paper, an improved mathematical model is proposed to analyze a special internal relationship between rainfall intensity and gas pollutants in urban atmospheric system, where the nonlinear relationship between precipitation and the concentration of pollutants in the air is considered, as well as the influence of random disturbances from the outside world. After the approximate solution of the system is obtained, the stability and bifurcation characteristics of the system with and without random disturbance are both analyzed. Theoretical analysis and numerical simulation results show that there is a close covariant relationship between rainfall and gaseous pollutants; the system has abundant bifurcation characteristics, which, in the physical sense, represents sudden changes of the gaseous pollutants in the urban atmospheric system; the urban atmospheric system can always be kept at a lower pollution level by applying slight disturbances to offset external disturbances.

- **Keywords:** Precipitation; Pollutant concentration; Nonlinear dynamic characteristics; Stochastic bifurcation

Xiaoxi Li, Jizhou Dong, Kaiqiang Jin, Qiangling Duan, Jinhua Sun, Min Li, Huahua Xiao. *Flame acceleration and deflagration-to-detonation transition in a channel with continuous triangular obstacles: Effect of equivalence ratio*. Pages 576-591.

Aiming to gain sufficient data to develop methods capable of predicting and evaluating the danger of potential explosion or even detonation hazards associated with industrial process piping systems, this paper experimentally studied the effect of equivalence ratio on flame acceleration and deflagration-to-detonation transition (DDT) of hydrogen-oxygen mixture in a channel equipped with continuous triangular obstacles. This obstruction can simulate the effect of continuous blockage or rough walls in process pipelines. High-speed schlieren photography and OH* chemiluminescence recording were used for visualization. Results show that significant vortex motion accelerates the delayed combustion between obstacles and generates strong jet flow to promote flame acceleration. DDT occurs when the equivalence ratio (Φ) is from 0.25 to 2.5. Minimum detonation initiation time and distance are obtained at Φ = 1.0 and 1.1. The equivalence ratio significantly influences DDT by affecting deflagration speed and shock strength. DDT mechanism for equivalence ratios closer to 1.0 is the survival of local detonation generated by intricate flame-shock interactions. While for equivalence ratios far from 1.0, i.e., extremely lean or rich fuel (Φ = 0.25, 2.0 and 2.5), DDT can be formed due to a combined effect of viscous heating at the boundary layer and preheat caused by shock compression.

- **Keywords:** Deflagration-to-detonation transition; Hydrogen-oxygen mixture; Continuous triangular obstacles; Equivalence ratio; Chemiluminescence recording; Shock-flame interaction

Jiajun Xie, Yiwei Zhong, Yu Yu, Mingyong Wang, Zhancheng Guo. Green capturing of Ag from ultra-low concentration precious metal wastewater by electrodeposition assisted with electrocoagulation: Electrochemical behavior and floc characterization. Pages 592-600.

As an environmental-friendly water treatment technique, direct electrodeposition (ED) encountered some difficulties to recover low-concentration metallic ions. This work proposed a novel electrodeposition assisted with electrocoagulation (ED-EC) process to remove and capture Ag+ from ultra-low concentration wastewater. Influences of operating parameters on the removal efficiency were investigated. Results showed that the Ag+ removal ratio of ED-EC increased to > 97.4 % compared to direct ED (<90 %), and Ag+ was reduced to < 0.1 ppm from an initial concentration of 2–20 ppm. Low current density, low pH and high Ag+ concentration improved electrodeposition, but weakened the formation and adsorption of the flocs by electrocoagulation. Aqueous Ag+ was captured and enriched in the flocs and the cathode deposit, where the Ag contents were > 3000 g/t and > 97 wt%, respectively. The economic assessment indicated that recovering Ag by ED-EC produced considerable benefits. Thus, this study provides meaningful guidance for resource recovery from precious metal wastewater.

- **Keywords:** Electrocoagulation; Electrodeposition; Precious metal wastewater; Ultra-low concentration; Resource recovery

Yan-Ru Wang, Jing-Ping Liu, Li-Ping Chen, Xing-Yu Shao, Sen Xu. *Thermal decomposition characteristics and runaway boundary conditions of HATO at adiabatic and high pressure situations*. Pages 601-608.

Dihydroxylammonium 5,5′-bistetrazole-1,1′-diolate (HATO) is a new generation of energetic material with low toxicity and high energy, which meet the needs of current

weapon systems. To explore the effect of particle size on the thermal stability and thermal risks of HATO, decomposition reactions of HATO nanoparticles (NPs) and microparticles (MPs) were studied by accelerating rate calorimeter. The two decomposition stages for HATO NPs and HATO MPs were researched and the apparent activation energies were obtained with different reaction order. Furthermore, temperature at the time of no return and self-accelerating decomposition temperature of the two kinds of HATO were calculated and discussed. Moreover, the thermal behaviors of HATO NPs at atmospheric and high pressure were researched by differential scanning calorimetry. The decomposition of HATO NPs was more violent at high pressure with higher peak power and the related thermokinetic parameters at the pressure of 1.0 MPa were identified.

- **Keywords:** Dihydroxylammonium 5,5′-bistetrazole-1,1′-diolate; Thermal decomposition; High pressure experiments; TNR; SADT

Lin Chen, Shan Ren, Xiangdong Xing, Jie Yang, Xiaodi Li, Mingming Wang, Zhichao Chen, Qingcai Liu. *Poisoning mechanism of KCl, K2O and SO2 on Mn-Ce/CuX catalyst for low-temperature SCR of NO with NH3*. Pages 609-619.

In this study, a series of K species or/and SO2 poisoned Mn-Ce doped CuX (MCCX) catalysts were prepared from waste blast furnace slag (BFS), and the influence mechanism of K species or/and SO2 poisoning on the catalysts in low-temperature NH3-SCR process was investigated. The results demonstrated that MCCX-KCl catalyst had poorer NO conversion than MCCX-K2O below 200 °C, and the co-existence of K species and SO2 considerably inhibited NO conversion. Aggregation of the Cu active component might also be facilitated by co-poisoning with K species and SO2. Furthermore, K species and SO2 co-poisoned catalysts showed fewer isolated Cu2+ species and Mn4+ species than that of K-poisoned catalysts, indicating a decrease in active sites after the addition of SO2. The co-effect of K2O/KCl and SO2 species impaired the redox capacity and decreased the surface acidity than K-poisoned catalysts to a greater extent. Nevertheless, K-poisoning had little effect on the surface intermediates during SCR reaction process, and K-poisoned catalysts followed both Langmuir-Hinshelwood (L-H) and Eley-Rideal (E-R) mechanism. However, MCCX-KCl-SO2 and MCCX-K2O-SO2 catalysts contained fewer nitrate species, indicating that the co-effect of K species and SO2 impeded the reaction between NO + O2 species and pre-NH3 species, thereby resulting in poor low-temperature NH3-SCR activity.

- **Keywords:** K or/and S poisoned catalysts; Blast furnace slag; Low-temperature NH3-SCR; Cu2+ active sites

Runze Yu, Yanyu Qiu, Huadao Xing, Mingyang Wang, Bin Li, Lifeng Xie. *Experimental study on the explosion characteristics of methane-air mixtures initiated by RDX in a rectangular venting chambre*. Pages 620-628.

ethane-air mixtures initiated by Hexogen (RDX) were experimentally investigated in a custom-designed rectangular venting device. By changing the methane concentration, the overpressure characteristics and flame propagation were studied under the conditions of RDX detonation and electric spark ignition, respectively. The results indicate that, compared with spark ignition, the RDX explosion shock wave leads to the structural vibration and interacts with the flame, shortening the methane reaction time and substantially increasing the explosion overpressure. When the methane concentration is close to the equivalence ratio of unity, only one pressure peak occurs after the vent plate opening. The pressure peak caused by the interaction between acoustic waves and flames, P3, appears only at methane concentrations of 8 vol% and 13 vol% under RDX

detonation. The acoustic vibration of the structure induced by different masses of RDX has a nonlinear impact on the increase of P3. The long reaction duration and the weakening of the shock wave result in a relatively small frequency of high-frequency oscillations at high concentrations.

- **Keywords:** RDX detonation; Overpressure; Flame development; Methane concentration; Explosion venting

Ting Li, Fang Zhu, Wenjing Liang, Guangyao Hu, Xiaoqiang Deng, Yongbin Xue, Jian Guan. *Simultaneous removal of p-nitrophenol and Cr(VI) using biochar supported green synthetic nano zero valent iron-copper: Mechanistic insights and toxicity evaluation*. Pages 629-640.

Nano zero-valent iron/copper bimetallic particles supported by peanut shell biochar were synthesized with green tea extracts (GT-BC@nZVI/Cu) and used for simultaneous removal of p-nitrophenol (PNP) and Cr (VI) from groundwater. GT-BC@nZVI/Cu was characterized by SEM, TEM, FTIR, XRD and XPS. The effect of pH, temperature, coexisting ions and humic acid on the removal of PNP and Cr (VI) were studied. Results showed that when pH value was 5 and the temperature was 313 K, the removal rates of PNP and Cr (VI) by GT-BC@nZVI/Cu reached 93% and 100 % within 30 min, respectively. Pseudo-first-order, pseudo-second-order and W-M models were used to analyze the experimental results. The adsorption isotherms of Langmuir and Freundlich were also evaluated. The analysis of these models shows that the pseudo-second-order kinetics and Langmuir adsorption isotherm can better describe the removal reaction of PNP and Cr (VI). The presence of coexisting anions (Cl-, SO42-, NO3- and CO32-) showed various effects on the removal of PNP and Cr(VI), while humic acid evidently inhibited the removal of PNP and Cr (VI). Moreover, the reusability of GT-BC@nZVI/Cu demonstrated that the removal of Cr(VI) and PNP are 62.45% and 47.32 % after three cycles, respectively. Mung bean seeds germinated 100% in both the GT-BC@nZVI/Cu suspension and the treated solution after 5 days of cultivation. The mechanism of Cr(VI) removal involves adsorption, reduction and co-precipitation. GC-MS analysis identified p-aminophenol as the reduced product and p-benzoquinone and hydroquinone as the oxidized product. These results demonstrated that the degradation of PNP is a combination of reduction and oxidation.

- **Keywords:** Green synthesis; Nano zero valent iron/copper; Biochar; Cr(VI); P-nitrophenol

Yitong Shao, Qi He, Yongsheng Fu, Geilu Zhang, Yiqing Liu. *Environmental impact and variation analysis of different CaO2 and Ca(NO3)2 dosing modes on microbial community in black-odorous sediment*. Pages 641-650.

CaO2 and Ca(NO3)2 are commonly used chemicals in the in-situ remediation of black-odorous sediments, but comparative studies on the impact on sediment microorganisms are scarce. This paper aimed to compare the impact of different CaO2 and Ca(NO3)2 dosing modes on microorganisms in black-odorous sediments. The results showed that CaO2 with single-dose in deep sediment performed best in removing nitrogen and phosphorus, while Ca(NO3)2 with multi-dose in shallow sediment was best in removing organic matter. After remediation, the abundance of sedimentary microbes increased significantly in each group. Microbial diversity in the CaO2 group decreased while it increased in the Ca(NO3)2 group. Proteobacteria and Firmicutes were the predominant microbes in black-odorous sediments. The relative abundance of Proteobacteria and Firmicutes raised in each CaO2 group, whereas Proteobacteria raised and Firmicutes declined in each Ca(NO3)2 group. Redundancy analysis demonstrated that microbes in black-odorous sediments were primarily influenced by NH3-N and COD in water.

FAPROTAX functional prediction revealed that the microbial functional gene of thiosulfate-respiration was significantly increased in the CaO2 group but decreased in the Ca(NO3)2 group. This research not only compares the impact of common chemicals on the microbial community of black-odorous sediments but also provides new data and findings for future in-situ remediation strategies of black-odorous sediments.

- **Keywords:** Black-odorous sediments; In-situ remediation; Calcium peroxide; Calcium nitrate; Pollutant removal; Microbial community

Yiyue Chen, Laibin Zhang, Jinqiu Hu, Chuangang Chen, Xiaowen Fan, Xinyi Li. *An emergency task recommendation model of long-distance oil and gas pipeline based on knowledge graph convolution network*. Pages 651-661.

When long-distance oil and gas pipeline accidents take place, a set of requirements and constraints ought to be considered, due to the various environment, multiple accident types and hazard-bearing bodies. Compliance with the response tasks directly influences the subsequent accident development. Furthermore, attribute to geographic location or communication limitations, the accident information may be delayed or unclear. Knowledge graphs are an advantageous representation of the fusion of complex relationships. On this basis, this study aims to establish an emergency task recommendation model that can adapt to several accident information description levels. Combined with the proposed emergency case framework, a knowledge graph of long-distance oil and gas pipeline emergency cases is established for the first time. Realize embedding learning by aggregating neighbor node and relationships. The accuracy of the emergency task recommendation is improved by introducing a variety of relations in the case-feature graph. Apply this model to the 11.22 Qingdao Oil Pipeline Explosion incident. Tasks such as culvert and well boundary detection, combustible gas concentration monitoring, and response upgrading are supplemented. Compare with the accident investigation report conclusions, the recommended tasks help to prevent the explosion. The proposed model not only has a case information recording framework but is also not bound by the input format of structured cases. It solves the issue of ambiguous case feature input in the task recommendation and has good practical application value.

- **Keywords:** Emergency decision support; Long-distance oil and gas pipeline; Emergency case framework; Emergency case knowledge graph; Knowledge graph convolution network; 11.22 qingdao oil pipeline explosion incident

Zhenran Wang, Tao Fu, Linrui Zhong, Yongsheng Fu, Yunlan Peng, Shixiang Wang, Yiqing Liu. *Synergistic effect of humic substances and bicarbonate on diclofenac degradation by Cu(Ⅱ)/peracetic acid*. Pages 662-670.

Bicarbonate (HCO3-) and humic substances (HS), two common water matrix components, were found to exhibit synergistic effect on diclofenac (DCF) degradation by Cu(Ⅱ)/peracetic acid (PAA) process in this work. The mechanism of their impacts on the performance of Cu(Ⅱ)/PAA system was systematically investigated and the reactive species generated in this system was identified. The results revealed that organic radicals ($CH_3C(O)OO\bullet$ and $CH_3C(O)O\bullet$) and Cu(Ⅲ) were both generated in HCO3--Cu(Ⅱ)-fulvic acid (FA)/PAA system, and the presence of FA induced Cu(Ⅲ) to become the dominant reactive species for DCF degradation. In comparison with humic acid (HA), FA showed a stronger enhancement effect on DCF removal in HCO3--Cu(Ⅱ)/PAA system, which might be due to its stronger electron transfer capability. However, DCF degradation in HCO3--Cu(Ⅱ)-HS/PAA system with HA-FA mixture was similar to that with HA alone, because Cu(Ⅱ) was prior to be coordinated with HA in HA-FA mixture. The operating parameters

(i.e., HCO3-, Cu(Ⅱ) and PAA concentrations) were optimized for DCF degradation. Finally, the efficient DCF degradation in real waters proved that the presence of HS and HCO3- in real waters also strongly enhanced DCF elimination by Cu(Ⅱ)/PAA process. The findings of this work suggested that HCO3- and HS, which are extensively distributed in aquatic environment, can significantly improve the performance of Cu(Ⅱ)/PAA system and this system may be an efficient technology for the removal of refractory pollutants in real waters.

- **Keywords:** Humic substances; Bicarbonate; Copper ion; Peracetic acid; Synergistic effect

Ming-Ting Lee, Bor-Yih Yu. *Evaluation on the intensified hydroxypropyl acrylate (HPA) production processes: Rigorous design, optimization, techno-economic and environmental analysis, and control*. Pages 671-685.

This work firstly proposed novel processes synthesizing hydroxypropyl acrylate (HPA) from diluted aqueous acrylic acid (AA) and propylene glycol (PG). As both AA and HPA dimerize, the key in process design is to hold the one-pass conversion low, and the product selectivity high. Herein, three process schemes using different strategies in enhancing selectivity, or handling recycle streams, were investigated. These include the conventional reaction/distillation configuration (Scheme 1), the intensified process using a side reactor (Scheme 2), or multiple side reactors with feed splitting (Scheme 3). After optimization, it was found that scheme 3 exhibits the greatest economic and environmental attractiveness, which reduces 43.4 % of cost, and 13.8 % of CO2 emission from scheme 1. From the optimized scheme 3, the minimum required selling price (MRSP) of HPA (Target: 20 % internal rate of return, or IRR) is in between 1.904 and 2.797 USD/kg under varying raw material prices (i.e. diluted AA= 0.566–1.140 USD/kg; PG = 1.148–1.403 USD/kg). These results reveal the improvement from the current technology of producing HPA (i.e. current price: 2.725 USD/kg). Finally, a control structure was proposed onto the optimized Scheme 3. It satisfactorily rejects the disturbances from feed flowrate, feed composition and catalyst deactivation.

- **Keywords:** Hydroxypropyl acrylate; Acrylic acid; Simulated annealing; Process intensification; Carbon emission; Process control

M. Zamani, E. Abbasi-Atibeh, J.S. Olfert, L.W. Kostiuk. *Co-flow jet diffusion flames in a multi-slot burner: Flow field and emissions*. Pages 686-694.

Motivated by the application of internally air-assisted flares and recent anomalous data that black carbon (BC) emissions changes are not monotonic with the amount of air added inside the fuel stream, a burner was designed to study the flow, emissions, and stability aspects of the existence of both normal and inverse jet diffusion flames in close proximity. Since the radius of curvature of a burner affects all aspects of combustion, such as dynamics, stability, flame structure, and emissions, a slot burner configuration, inspired by the Wolfhard-Parker burner, was adopted. This multi-slot burner consists of five parallel rectangular slots (i.e., the central slot for the inner air, sandwiched between two fuel slots, and surrounded by two outer air slots). When operated with laminar fuel and air flows, this burner produced flame sheets at each fuel-air mixing layer with open optical access to all the flows. Flow fields were characterized using two-dimensional two-component particle image velocimetry, while simultaneous single-lens reflex photography was used to establish the overall height and the location of the flames. Emission measurements specifically targeted BC, a precursor of soot, and oxides of nitrogen (NOx). The experimental test conditions involved constant flows of outer air and propane, and variable inner air flow. At one extreme, i.e., zero inner air flow, two flame bases

were produced at the interfaces between the fuel and outer air streams. These flames merged to produce a normal diffusion flame. With the addition of inner air, two more flame bases appeared (referred to as the inner flame) and formed an inverse diffusion flame. With increasing inner air flow, the inner flame transitioned from a closed-tip flame, to an open-tip flame, and eventually to a lifted flame. With increasing inner air flow, the NOx emissions remained constant while the BC emissions, which were 3 g/kg-fuel with no inner air, rose by an order of magnitude as it became an open-tip flame. Only when the inner flame finally lifted off due to the inner air flow, did the BC emissions collapse to near zero. Phenomenological models associated with the importance of partial premixing were proposed to explain this collapse, thereby generalizing this finding to other combustion systems when attempting to reduce BC emissions through secondary internal air addition.

- **Keywords:** Normal and inverse jet diffusion flame; Multi-slot burner; Particle image velocimetry; Emission index; Black carbon; Lift-off

Hua-Wei Chen, Yu-Lin Kuo, Chien-Hua Chen, Chyow-San Chiou, Wei-Ting Chen, Yi-Hung Lai. *Biocompatibile nanofiber based membranes for high-efficiency filtration of nano-aerosols with low air resistence*. Pages 695-707.

Particulate matter (PMs) from combustion emissions (traffic, power plant, and industries) and the novel coronavirus (COVID-19) pandemic have recently enhanced the development of personal protective equipment against airborne pathogens to protect humans' respiratory system. However, most commercial face masks still cannot simultaneously achieve breathability and high filtration of PMs, bacteria, and viruses. This study used the electrospinning method with polyimide (PI) and polyethersulfone (PES) solutions to form a nanofiber membrane with low-pressure loss and high biocompatibility for high-efficiency bacteria, viruses, and nano-aerosol removal. Conclusively, the optimized nano-sized PI/PES membrane (0.1625 m2/g basis weight) exhibited conspicuous performance for the highest filtration efficiency towards PM from 50 to 500 nm (99.74 %), good filter quality of nano-aerosol (3.27 Pa−1), exceptional interception ratio against 100-nm airborne COVID-19 (over 99 %), and non-toxic effect on the human body (107 % cell viability). The PI/PES nanofiber membrane required potential advantage to form a medical face mask because of its averaged 97 % BEF on Staphylococcus aureus filiation and ultra-low pressure loss of 0.98 Pa by referring ASTM F2101–01. The non-toxic PI/PES filters provide a new perspective on designing excellent performance for nano-aerosols from air pollution and airborne COVID-19 with easy and comfortable breathing under ultra-low air flow resistance.

- **Keywords:** Electrospinning method; Polyimide; Polyethersulfone; Nano-sized PI/PES membrane; Medical face mask