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Hongpeng Lv, Depeng Kong, Ping Ping, Gongquan Wang, Hengle Zhao, Xinyi Dai. *Anomaly detection of LiFePO4 pouch batteries expansion force under preload force*. Pages 1-11.

Overcharging, overheating and other abnormal conditions are important causes of thermal runaway of Li-ion batteries, and a major safety issue for Li-ion batteries. Therefore, it is critical to detect these faults as soon as they are triggered. In this paper, the actual usage scenario of the battery was simulated by setting the appropriate preloading force. And the characteristics of the changes of the battery expansion force under abnormal conditions were studied by battery charging and discharging, overcharging, overdischarging and thermal runaway experiments. In particular, we proposed a fast and high confidence battery fault detection method by the characteristics of the expansion force change under various faults, which could provide early warning of multiple faults. This work provided a reliable method of detecting battery failures at an early stage and ensured process safety and reduced environmental pollution caused by lithium-ion battery accidents through reasonable fire prevention measures.

- **Keywords:** LiFePO4; Detection; Expansion force; Electricity abuse; Thermal runaway

Suresh Vellaiyan. *Bauhinia racemose seeds as novel feedstock for biodiesel: Process parameters optimisation, characterisation, and its combustion performance and emission characteristics assessment with water emulsion*. Pages 12-24.

Second-generation biofuels produced from inedible feedstocks may be a viable alternative to diesel fuel and the transformation of the seeds into biodiesel has been the subject of some exciting studies in the Bauhinia family. However, none of the studies attempted to optimise the transesterification process parameters of Bauhinia racemose biodiesel (BRB) for a higher yield rate and analyse the BRB compatibility with water emulsion. The current research thereby optimises the process parameter variables for a higher yield rate of BRB, characterises the fuel, and explores the effect of water emulsion in BRB on combustion, performance, and environmental features. The transesterification

process was started with a reusable catalyst, and its various parameters were optimised to achieve maximum efficiency. The optimal input parameters, according to the optimisation are a molar ratio of 8.11:1, a reaction temperature of 66.04 °C, and a reaction time of 115.2 min; under these conditions, the yield rate of BRB is 92.9%. The Fourier-transform infrared spectroscopy examination suggests that the carbon-based elements of the developed BRB appear to be in excellent order, and according to data from gas chromatography–mass spectrometry, methyl esters contribute most significantly. The plain diesel (PD) was first blended with 10%, 20%, and 30% volume of BRB, and then 5% and 10% volume of water were added to the 30% BRB-blended PD. The experiments were carried out in a diesel engine under various operating conditions. Maximum in-cylinder pressure is 3.4% lower for PD that has been blended with 30% BRB, while it is 2.41% higher when 10% water is added. Both the rate of heat release and the time it takes to burn is reduced in BRB blends of PD and water-emulsified fuels. Adding 30% BRB mixed PD decreases brake thermal efficiency (BTE) by 3.2%, and 10% water-emulsified BRB improves BTE by 3.9%. When BRB is used with PD, all emissions are mitigated, except for oxides of nitrogen (NOx). NOx emissions can be reduced by 12.1% when fuel is emulsified in 10% water. In addition, the proposed fuel mixture will reduce demand for regular diesel fuel by about 40%.

- **Keywords:** Waste-to-Energy; Bauhinia racemose biodiesel; Process optimisation; Fuel characterisation; water emulsion; Energy and environmental assessment

Jamasb Pirkandi, Mostafa Mahmoodi, Ali Shirinfekr, Erfan Ebadati. *Parametric study and thermodynamic performance analysis of a hybrid solid oxide fuel cell-Stirling engine system for cogeneration applications*. Pages 25-39.

Given the increase in global energy consumption, the scarcity of fossil fuel resources, and the rise in environmental pollution have necessitated the use of novel technologies in energy production. Among these technologies, fuel cells have attracted researcher's attention due to their low environmental pollution, high efficiency, and ability to be combined with other power generation systems. The present research studies the performance of a hybrid solid oxide fuel cell-Stirling engine (SOFC-ST) system from a thermodynamic perspective. To this end, the fuel cell and the Stirling engine were modeled via coding in MATLAB software. The decision variables in this analysis were the current density, fuel utilization factor, fuel flow rate, number of fuel cells, air flow rate, and type of fuel used in the fuel cell. According to the results, when hydrogen is used as the fuel in the fuel cell, its power generation increases from 60 kW to 67 kW and its efficiency rises from 44.2 % to 49.4 % with the addition of the Stirling engine. However, if the fuel is methane, the power generated by the fuel cell increases from 19.9 kW to 26.6 kW, while its efficiency increases from 36.9 % to 49.2 %.

- **Keywords:** SOFC; Stirling engine; Hybrid system; Energy Production

Thomas Dippong, Cristina Mihali, Monica Marian, Oana Mare Rosca, Maria-Alexandra Resz. *Correlations between chemical, hydrological and biotic factors in rivers from the protected area of Tisa Superioară, Romania*. Pages 40-55.

This paper aimed to evaluate the water quality of several rivers (Șugătag, Sapanta, Isa, Vișeu and Tisa), vegetation and fish population in the protected area of ROSCI0251Tisa Superioară, Romania to determine the extent to which the anthropic activities (tourism activities and livestock) affect the water characteristics and implicitly it's quality. Results indicated contamination with NH4+, Fe, Ni, Cr and Mn, with values ranging from 0.14 to 0.83 mg/L NH4+, 0.07–0.76 mg/L Fe, 2.9–31 mg/L Ni, 1.38–59 mg/L Cr and 7.6–127 mg/L Mn, caused by anthropogenic activities. According to the pollution indices

scores, samples were characterized by low, medium, and high pollution levels. HPI (Heavy metal Pollution Index) and HEI (Heavy metal Evaluation Index) scores ranged between 21.6 and 54.4 and 1.5–8.4, respectively. Risk assessment indicated no risks at metals through ingestion or dermal contact. The chronic daily intake ranged between 9.08 × 10−6 and 2.09 and the hazard quotient ranged between 9.61 × 10−7-3.45 in both dermal and ingestion pathways. The fish population included 23 species. The ichthyofaunal assessments indicated good quality and stability. This study provides important data for the riparian population, researchers, and even policymakers, regarding the quality status and potential pollution degree of surface waters in the protected area of Tisa.

- **Keywords:** River; Statistical analysis; Quality assessment; Health risk assessment; Heavy metal pollution indices

Feihao Zhu, Zegong Liu, Yunfei Zuo, Na Yang, An-Chi Huang. *Damage and failure characteristics of coal and surrounding rock under shaped blasting*. Pages 56-64.

The high crustal stress in deep coal mining undermines the efficiency and safety of blasting operations conducted to increase gas permeability in the coal seam. Therefore, in this study, theoretical research, computer-based numerical simulations, and experiments were conducted to investigate the damage and fracture characteristics of a coal body and surrounding rock subjected to shaped blasting. ANSYS LS-DYNA was employed for numerical simulations to understand how a shaped jet is formed and how damage occurs in shaped blasting. A model of crack evolution under the influence of detonation gases that is based on fracture mechanics theory was constructed to analyze the mechanism underlying the directional propagation of detonation cracks in shaped blasting. In the conducted experiments, shaped blasting resulted in the creation of an oval-shaped fragmentation area, which was evidence that the shaped cartridge limited the loss of energy in fragmentation, allowed detonation cracks to evolve further in the specimen, and caused the formation of a main crack that propagated in the direction along which energy was concentrated (i.e., directional damage). Compared with ordinary blasting, shaped blasting facilitated more efficient blast energy use and reduced undesirable blast disturbance to the surrounding rock by 58% according to the computed tomography image of resistivity. The results of this study provide valuable insights on safe and efficient coal production.

- **Keywords:** Deep mining; Shaped blasting; Crack evolution; Disturbance to wall rock; Damage detection

Ali Ekramipooya, Mehrdad Boroushaki, Davood Rashtchian. *Application of natural language processing and machine learning in prediction of deviations in the HAZOP study worksheet: A comparison of classifiers*. Pages 65-73.

The HAZOP (Hazard and Operability) study is one of the most well-known approaches in process hazard analysis. The HAZOP study is a systematic procedure a multidisciplinary team uses to find hazards and operability issues through brainstorming. The conventional HAZOP study requires much time, is also knowledge-intensive, and is susceptible to human mistakes. Therefore, there is a significant incentive to automate the HAZOP study. This study investigated the effectiveness of Natural Language Processing (NLP) and Machine Learning (ML) in HAZOP study automation. The case study used in this contribution is based on a conventional HAZOP study report. Initially, the causes were converted into feature vectors using NLP's simple sentence embedding technique (Bag of Words). Random oversampling was employed to manage the limited and imbalanced dataset. Finally, ML classifiers such as Decision Tree, linear Support Vector Machine,

Random Forest, Logistic Regression, Gaussian Naïve Bays, and K-Nearest Neighbors were applied to predict deviations. Decision Tree outperformed other classifiers with 92% accuracy. This study's integrative approach applies even to small units and companies with limited training datasets. This is because it does not require a large training dataset.

- **Keywords:** Chemical process safety; Process hazard analysis; HAZOP study automation; Natural language processing; Machine Learning

Xiaoyang Luan, Muchen Zhang, Shuaiyu Zhao, Bin Zhang. *Numerical study on the effects of bund on liquid pool spreading and vapor dispersion after a catastrophic LNG tank failure*. Pages 74-86.

Liquefied natural gas (LNG) storage tanks are usually equipped with bunds to provide an additional layer of protection. However, the catastrophic failure of an LNG storage tank usually results in a bund overtopping. The overtopped LNG will evaporate rapidly at ground surface to form the flammable gas cloud. Previous studies have developed computational fluid dynamics (CFD) models to investigate the ability of bunds to retain liquids; However, the models were developed based on ambient liquid, ignoring the evaporation phenomena and vapor dispersion of LNG. In this work, a multiphase CFD model which integrated with the evaporation model was proposed to simulate the complete overtopping process (including LNG overtopping, LNG spread, LNG evaporation and vapor dispersion). The data from two field experiments were used to validate the model. In addition, this paper studied a case of catastrophic failure that derived from an industrial LNG Tank. The effect of the bund configurations on the wind flow field, the overtopping fraction, the spread of LNG and the dispersion of LNG vapor cloud was analyzed. The present work can help relevant personnel to better assess the engineering risks associated with catastrophic failure of storage tanks for decision making in the process safety framework.

- **Keywords:** LNG; Catastrophic failure; Bund overtopping; Vapor dispersion; CFD

Nima Arast, Mehrdad Farhadian, Shahram Tangestaninejad, Amir Hossein Navarchian. *Efficient photocatalytic performance of BiVO4/ ZIF-8 /Cu2S/Ag2S incorporated in solar driven-cleaning ABS/MWCNT membrane applied in metronidazole decontamination*. Pages 87-100.

To take advantage of solar energy, BiVO4/ZIF-8/Cu2S/Ag2S quaternary photocatalyst with different amounts of ZIF-8 was synthesized. Composites were characterized by FTIR, XRD, TEM, HR-TEM, PL, EDX, DRS and BET. The photocatalytic performance was evaluated and composite with 77.5, 15, 5 and 2.5 wt% of BiVO4, Cu2S, Ag2S and ZIF-8 showed the best qualification with 83.5 % metronidazole removal efficiency. Photocatalytic nanoparticles were incorporated into ABS/MWCNT membranes and they were characterized by SEM, EDX, AFM, electrical conductivity and contact angle measurements. The membrane with 2 wt% MWCNT had conductivity 106 times higher than that of pristine ABS membrane. The contact angles were decreased and the membrane with a more hydrophilic surface resulted in the flux improvement to 200 kg/m2. h. The enhanced drug retention up to 81 % indicated that by using the proper amount of photocatalyst it was possible to increase both the flux and rejection parameters. The flux recovery after solar illumination was obtained as 95.6 % for membrane with 0.5 wt% photocatalytic composites, that result in appropriate anti-fouling capability. finally, high performance photocatalytic activity makes membrane with 0.5 wt% photocatalyst and 1 wt% MWCNT superior for long-life filtration (36 h).

- **Keywords:** ABS membrane; BiVO4/ ZIF-8/Cu2S/Ag2S photocatalyst; Flux recovery; Solar cleaning; Water decontamination

Jun Xie, Jiapeng Li, Jinghong Wang, Juncheng Jiang, Chi-Min Shu. *Fire risk assessment in lithium-ion battery warehouse based on the Bayesian network.* Pages 101-114.

Because of the instability and susceptibility to thermal runaway of lithium-ion batteries (LIBs), their storage has always been at high risk of fire. Numerous studies have analyzed the risk of fire in lithium-ion battery (LIB) warehouses. Still, most of them have focused on the factors influencing the fire following the thermal runaway of a LIB occurs, and there has been a lack of research on the causes of the LIB thermal runaway being occurred. To address this shortcoming, this paper proposed a comprehensive framework considering multiple influencing factors for fire risk assessment in LIB warehouses that combines Bayesian networks (BNs) and expert evaluation. The proposed framework adopts the Bayesian network (BN) model that considers three main types of parameters: fire causes, fire spread influencing factors, and fire consequences. The main objective was to analyze the evolution and consequences of LIB warehouse fires dynamically and provide effective suggestions for fire risk reduction. The results showed that the proposed framework was a reliable avenue for fire risk assessment of LIB warehouses. In addition, it was demonstrated that human factors commonly cause the LIB warehouse open fires. Thus, to prevent open fires from continuing spreading, the LIB warehouses should avoid storing batteries with high state of charge values; furthermore, if it is necessary to store them, automatic sprinklers and other firefighting facilities should be installed. In addition, timely firefighter response and the installation of mechanical ventilation systems are essential to substantially curtail casualties.

- **Keywords:** Thermal runaway; Multiple influencing factors; Expert evaluation; BN model; State of charge

Abdul Naeem, Tooba Saeed, Murtaza Sayed, Bashir Ahmad, Tahira Mahmood, Muhammad Farooq, Fouzia Perveen. *Chitosan decorated zirconium metal-organic framework for collaborative adsorption and photocatalytic degradation of methylene blue and methyl orange*. Pages 115-130.

A type of crystalline porous material known as zirconium metal-organic frameworks (UiO-66) is made up of organic carboxylate ligands and inorganic zirconium clusters. The UiO-66 has consistent pore sizes, large porosities, exceptional adsorption capabilities, and particular functional groups for increasing dye adsorption. This study reports the synthesis of Zirconium metal-organic framework (UiO-66) and chitosan composite of zirconium metal−organic framework (CS/UiO-66) for potential adsorption of methyl orange (MO) and methylene blue (MB) dyes from the aqueous media and additional, excellent photodegradation capability of the synthesized material towards selected dyes. The synthesized materials were successfully characterized for structural, morphological, surface and thermogravimetrical analysis. The exclusion of dyes onto the CS/UiO-66 followed the trend MB (2321 mg/g) > MO (900 mg/g) respectively. The maximum sorption and degradation capacity of the CS/UiO-66 were increased by 5–10 times after its composite with chitosan (CS) and the affinity of the dyes towards the different adsorbents followed the sequence CS/UiO-66 > UiO-66 > CS which is parallel to their surface properties. The negative values of the entropy i.e., − 382 for MB and − 249 for MO affirmed the controlled versatility of the MO, and MB onto CS/UiO-66 whereas the isosteric heat of adsorption i.e., − 201 kJ/mol for MB and − 153 kJ/mol for MO illustrated the exothermicity of the adsorption process. The intraparticle diffusion and Richenberge kinetic models demonstrated that pore diffusion dominates in the adsorption of MB while film diffusion has a greater involvement in the MO adsorption of CS/UiO-66. Moreover, the photocatalytic degradation study indicated that the pH and H2O2 play a significant part in the deprivation of dyes. While GC-MS analysis revealed that the photocatalytic degradation of MB resulted in the formation of six TPs. The toxicity of these TPs of MB

was evaluated by ECOSAR program and the results showed that the TPs were less toxic than the parent MB molecule.

- **Keywords:** Adsorption; Chitosan; Methylene Blue; Methyl Orange; Metal Organic Framework; Photocatalytic Degradation

Jun Hou, Shihang Li, Shuda Hu, Hui Cheng, Muze Han, Changgeng Gui, Qiaosong Guo, Liang Yuan, Fubao Zhou. *Research and application of self-powered induction spray dust removal system for long-distance belt conveying in underground coal mines*. Pages 131-139.

A self-powered induction spray dust removal system for long-distance belt conveying in underground coal mines was developed. In the system, the kinetic energy of the conveyor belt can be converted into the electrical energy required by the infrared sensing atomization spray device. When the rotational speed of the roller reaches 230 r/min, 12.33 V electricity can be steadily generated. Further proposed to install multiple sets of dust reduction systems with an optimal spacing of 240 m. The effectiveness of this installation method was verified by turning systems on one by one in the 25211 transportation roadway of the Hongliulin coal mine. The total dust concentration was reduced from 11.78 mg/m3 to 3.88 mg/m3, and the respirable dust concentration was reduced from 6.33 mg/m3 to 2.48 mg/m3. The results show that the developed self-powered induction spray dust removal system can dramatically improve the long-distance belt conveying environment in coal mines.

- **Keywords:** Self-powered; Induction spray; Dust removal; Long-distance belt conveying

Junying Song, Xiaofei Ren, Guicong Hu, Xiaolong Hu, Weimin Cheng. *Enhanced PMS activation by MOF-derived Co3O4/sepiolite composite for norfloxacin degradation: Performance, mechanism and degradation pathway*. Pages 140-154.

In this study, cobalt metal-organic framework (Co-MOF) derived Co3O4/sepiolite hybrid catalyst was prepared by a facile wet chemical method followed by the calcination crystallization process. In Co3O4/sepiolite composite, Co3O4 nanoparticles with smaller grain size were well dispersed on sepiolite surface. The larger reaction rate constant was obtained in Co3O4/sepiolite/PMS system for norfloxacin (NFX) degradation (0.2588 min−1), which was almost 3.44 times that in Co3O4/PMS. The greatly enhanced NFX degradation performance was mainly ascribed to the combination of Co-MOF precursor and sepiolite support resulting in higher adsorption capacity, more exposed reaction active sites and overspreading surface hydroxyl groups. The electron paramagnetic resonance (EPR) and quenching experimental results indicated that the radical and non-radical pathway were responsible for the NFX degradation, and the SO4•- and 1O2 were the major contributors. Moreover, the continuous redox cycle of Co(III)/Co(II) and the surface -OH on catalyst played the important roles in the continuous production of the reaction active species thereby achieving the efficient degradation for NFX. In addition, the enhanced catalytic mechanisms and NFX degradation pathways were proposed. Overall, our study provides new insights for designing and developing efficient and environmentally friendly catalysts for practical wastewater treatment via activating PMS.

- **Keywords:** MOF precursor; Co3O4; Sepiolite; Peroxymonosulfate; Norfloxacin

Hao Huang, Rui Wang, Kun Zhou, Lu Ning, Kai Song. *CausalViT: Domain generalization for chemical engineering process fault detection and diagnosis*. Pages 155-165.

Fault detection and diagnosis (FDD) is a promising technology for safe operation, quality control, and profitability improvement in chemical process systems. In practice, chemical process systems usually switch among operating conditions in response to market demands, fatigue, malfunctions of components and environments. However, FDD models often deteriorate when transferred from one operating condition to another. Current widely used FDD models are trained and tested in identical domains (or operating conditions) without emphasis on the capability of domain generalization. Furthermore, they ignore the causality that remains invariant among domains but excessively rely on statistical correlation that varies from domain to domain. This paper presents an FDD model named CausalViT. Causality and a gradient reversal operation are designed to enhance domain generalization. In CausalViT, a Causal Layer is constructed to discover the causal mechanism in features to purify superfluous domain-specific statistical correlation. Then, a domain classifier cooperating with gradient reversal layers is developed to further enhance the domain invariance. To evaluate the CausalViT, comparisons have been made between it and other advanced FDD models in six domains/modes in Tennessee Eastman Process. CausalViT shows superiority from the perspectives of both fault detection ratio and domain generalization, obtaining an average 16% improvement on domain generalization. Dimension reduction visualization shows the significance of domain generalization and gives a deeper insight into CausalViT. Furthermore, the convergence of the model and the effectiveness of components in the model have been analyzed and demonstrated.

- **Keywords:** Causality inference; Domain generalization; Fault Detection and Diagnosis; Gradient reversal operation; Tennessee Eastman process; Transformer

Zhuo Liu, Rongxin Guo, Xiao-Yong Wang, Chaoshu Fu, Run-sheng Lin. *Construction ceramsite from low-silicon red mud: Design, preparation, and sintering mechanism analysis*. Pages 166-179.

Low-silicon red mud (LSRM) is limited in its application in the field of light aggregates for construction. Supplementation sintering materials (SSMs) effectively aids LSRM in preparing sintered construction ceramsite. To produce an LSRM-based ceramsite with economical and effective performance, this study investigated the effect of SSMs (silica fume, bentonite, and glass powder) on the performance of the ceramsite and determined the optimum ratio using the response surface method (RSM). The results indicated that the silica fume (SF) significantly influenced the apparent density (AD) and water absorption (WA) of the ceramsite; with an increase in SF, AD increased and WA decreased. SF and glass powder (GP) were negatively correlated with particle strength (PS), whereas bentonite was positively correlated with PS. The optimum doping values for SF, bentonite, and GP were determined as 19.79, 9.28, and 12 wt%, respectively. Ceramsite could achieve the best performance with an AD of 1254 kg/m3, a WA of 3.13%, and a PS of 13.1 MPa. In addition, the formation of aluminosilicate played a positive role in the fixation of heavy metals and the reduction of the pH value of ceramsite, ensuring its good environmental performance.

- **Keywords:** Waste utilization; Construction ceramsite; Low-silicon red mud (LSRM); Supplementary sintering materials (SSMs); Response surface methodology (RSM); Environmental performance

Roshanak Pishbin, Toraj Mohammadi, Maryam Ahmadzadeh Tofighy. *PVDF ultrafiltration membranes containing copper oxide-charcoal based graphene oxide nanohybrids with enhanced performance and antifouling properties*. Pages 180-195.

Charcoal based graphene oxide-copper oxide (GO-CuO) nanohybrids were successfully synthesized via the co-precipitation method. It was then used to improve polyvinylidene fluoride (PVDF) ultrafiltration (UF) membrane properties and performance. The PVDF/GO-CuO UF nanocomposite membranes containing different contents of the synthesized GO-CuO nanohybrids were prepared via the phase inversion method. It was found that hydrophilicity of PVDF membrane containing 0.2 wt% of the synthesized GO-CuO nanohybrids increases than the neat PVDF membrane, so that its water contact angle (WCA) decreases from 80.68±1.23° for the neat PVDF membrane to 60.53±5.25° for the modified membrane containing 0.2 wt% of the synthesized GO-CuO nanohybrids. On the other hand, compared to the neat PVDF membrane, pure water flux (PWF) of this modified nanocomposite membrane increases by about 77% (from 101.1±1.82 to 178.87±1.47 LMH) and exhibits 94.28±0.93% rejection of bovine serum albumin (BSA). This improvement is due to increased hydrophilicity, porosity, average membrane pore size, and decreased membrane surface roughness. The results of fouling measurements showed 42%, 60%, and 8% reduction in total fouling ratio (Rt), irreversible fouling ratio (Rir), and reversible fouling ratio (Rr), respectively. This indicated that antifouling properties of the modified membrane is significantly improved. It was found that the fabricated PVDF/GO-CuO nanocomposite membrane exhibits better performance than the neat PVDF membrane. Also, the results showed that this membrane also exhibits better properties and performance than the PVDF/GO and PVDF/CuO nanocomposite membranes. Therefore, it can be concluded that the fabricated PVDF/GO-CuO nanocomposite membrane has excellent potential for water and wastewater treatment applications.

- **Keywords:** Ultrafiltration membrane; Polyvinylidene fluoride; Graphene oxide-copper oxide nanohybrids; Fouling; Water treatment

Xinzhi Zang, Qun Wang, Huihui Sun, Wei Liu, Zhen Li, Chunzhi zheng, Zhaolian Ye, Songjian Zhao. *Excellent degradation of toluene by non-thermal plasma coupled with M-BTC MOF (M=Mn, Cu, Ce)*. Pages 196-206.

In view of the unsatisfactory synergy between plasma technology and catalyst, a series of M-BTC MOFs (M=Mn, Cu, Ce) were introduced to couple with non-thermal plasma using for toluene degradation. M-BTC MOFs containing multi-carboxylic groups were successfully synthesized and presented the excellent crystallinity, morphology and thermal stability. DBD-catalysis systems presented the more excellent toluene degradation performance than single DBD alone system. Due to the porous structure and the multivalent form of manganese, the highest toluene degradation efficiency of 96.27%, the energy efficiency of 22.32 g/kW·h, the CO2 selectivity of 53.5% and the mineralization degree of 70.17% were acquired for DBD coupled with Mn-BTC under SED of 766.35 J/L. Besides, DBD/Mn-BTC had the lowest ozone and NOx production. Moreover, the toluene degradation mechanism was analyzed by plasma emission spectra analysis, XPS spectra and GC-MS diagram analysis. It indicated plasma discharge can produce abundant free radicals and reactive species to decompose toluene firstly, and the residual toluene and intermediates in the gas can be then adsorbed on Mn-BTC and further oxidized by metal active species. Furthermore, more reactive oxygen species will be generated by activating ozone through Mn-BTC, which was beneficial for toluene degradation.

- **Keywords:** Toluene degradation; DBD; Mn-BTC; Catalyst

Naveen Malik, Sudarshan Singh Lakhawat, Vikram Kumar, Vinay Sharma, Jasvinder Singh Bhatti, Pushpender Kumar Sharma. *Recent advances in the omics-based assessment of microbial consortia in the plastisphere environment: Deciphering the dynamic role of hidden players*. Pages 207-225.

Continuous disposal of plastic waste and its accretion in the environment is the biggest challenge the world has ever faced. Breaking its terrestrial bounds, plastic waste has now extended its outreach to aquatic territories including marine ecosystems. Photooxidation-mediated partial degradation converts plastic polymers to micrometric dimensions, thus augmenting their biomagnification in the food chains. Besides contaminating the food chains, microplastics also act as potential carriers of pollutants and pathogenic microbes. The slow and inefficient biodegradation of plastic by microorganisms in their natural habitats offers an opportunity to explore biotechnological interventions to overcome and mitigate the hazardous effects of plastic waste. Microorganisms utilize plastic polymer as a carbon source thus deriving energy from its oxidation and mineralization. The whole microbial consortium in the plastisphere interacts during the biodegradation process. The emergence of these novel plastic-dwelling microbial communities makes plastic degradation a very complex and finetuned process, where the expression of novel plastic-degrading genes and resultant pathways and interaction networks all contribute towards biodegradation. Thus, it is quite challenging to study such vast consortia of microbial communities by conventional approach to fully understand the degradation pattern of plastics. The techniques like shotgun metagenomics, transcriptomics and meta transcriptomics, next-generation amplicon sequencing, proteomics and metaproteomic, etc. have been successfully employed in recent years for identifying novel microbial species, gene pool, interactions network, and reaction pathways from different microbial consortia. Among several classes of bacteria, the Flavobacteriaceae, Rhodobacteriaceae, and Phycobactereaceae have shown their remarkable presence in different plastisphere. Omics approaches have also revealed high-level expression of plastic-degrading enzymes like esterases, depolymerases, hydrolases, and reductases. The applicability of these techniques in context to the studies of microbiota in the degradation of plastics is defined by their high accuracy, quickness, and sensitivity. The current review accentuates the significance of omics-based studies in identifying specific microbiota, dynamic gene pool, functional pathways, and metabolic networks of the plastisphere microbial consortia.

- **Keywords:** Metagenomics; Meta transcriptomics; Plastic pollution; Pollutants; Pathogens; Microbial dynamics

Matteo Iaiani, Alessandro Tugnoli, Valerio Cozzani. *Process hazard and operability analysis of BPCS and SIS malicious manipulations by POROS 2.0*. Pages 226-237.

The increasing interconnectivity with external networks and the higher reliance on digital systems make the facilities of the chemical, process, and Oil&Gas industry more vulnerable to cyber-attacks. These attacks have the potential of causing events with severe consequences on property, people, and the surrounding environment such as major event scenarios. The application of the currently available methodologies for cyber risk identification to complex plants with a large number of units may be demanding and cumbersome. The present study proposes an updated methodology, named POROS 2.0, that allows reducing time and effort in application by limiting the scope of the analysis to relevant cybersecurity scenarios. The latter are identified by investigating the potential escalation of consequences propagating among process and/or utility nodes of the manipulations of BPCS and SIS, similar to what is done in the HazOp technique in the safety domain. POROS 2.0 was demonstrated by the application to a case study addressing a fixed offshore platform for gas exploitation.

- **Keywords:** Cybersecurity; Cyber risk; Hazard identification; Chemical and process industry; Methodology; Cyber-attack

Yu Ouyang, Guangyong Zeng, Wei Zhu, Xuemei Yao, Mengyun Yang, Xiuyu Long, Jie Zheng, Yaping Tao, Yaocheng Deng, Chunxia Ding. *Highly efficient catalytic degradation of dicamba using Fe3O4/montmorillonite composite: Mechanism and toxicity assessment*. Pages 238-248.

Dicamba (DIC) posed significant hazards to aquatic environment owing to its toxic and refractory property in agricultural production, which has been paid increasing concern. Herein, a novel magnetic montmorillonite composite (Fe3O4/Mt) was fabricated for catalyzing peroxymonosulfate (PMS) to decompose DIC. The results exhibited that 3.0 mM PMS and 2.0 g/L Fe3O4/Mt could decompose nearly 90% of DIC, and the removal efficiency of DIC stayed above 66% after 10 cycles. The electron spin resonance tests and quenching experiments revealed that SO4•− and •OH were the main active radicals responding for DIC degradation. Moreover, based on the density functional theory (DFT) calculations and LC-MS, C1, C2, C4, and C5 atoms of DIC with high electrophilic activity were prone to be attacked by radicals, and were ultimately decomposed into five degradation intermediates. Finally, the toxicity assessment proved that most of the intermediates exhibited lower toxicity levels than that of DIC. These findings demonstrated that Fe3O4/Mt was a recyclable, stable, and safe catalyst for activation PMS to decompose persistent organic pollutants in contaminated water.

- **Keywords:** Montmorillonite; Fe3O4; Degradation; DFT calculation; Toxicity assessment

Zongling Zhang, Wei Gao, Yonghao zhou, Kai Zhang, Haipeng Jiang. *Characteristics of nano-PMMA dust explosion through the vented tube*. Pages 249-259.

The explosion venting experiments of 150 nm polymethyl methacrylate (PMMA) dust with different lengths (L) and diameters (D) of the vent tube are conducted. The effect of tube size on overpressure and flame propagation behavior is explored. High-frequency and low-frequency Helmholtz oscillations are observed on the overpressure curves in the chamber. The (dP/dt)max in the chamber is increased with high-frequency oscillations, while the maximum flame width is also visible with low-frequency Helmholtz oscillations. As the L increases from 0 m to 2 m, the Pred,max increases by 29.2–145.1% and the (dP/dt)max increases by 38.4% – 127.7%. With the increase of the D, the Pred,max in the chamber and vent tube decreases, and the flame transforms from an under-expansion jet flame to a subsonic jet flame. Due to the interaction between the external flow field and the concentration of unburned particles, the maximum external overpressure increases alongside with the incease of the tube length and diameter. In addition, the maximum calculation error of EN14491 is 1100%, while NFPA68 seriously underestimates the explosion venting pressure. A modified prediction model is established to provide a design method for a safe vent through the vent tube of the nano-dust explosion.

- **Keywords:** Nano-dust explosion venting; Pressure characteristics; External flame; Pressure predictions

Tao Hai, Jincheng Zhou, Yazen S. Almashhadani, Rishabh Chaturvedi, Abdullah H. Alshahri, Hamad R. Almujibah, Ahmed Sayed Mohammed Metwally, Mirzat Ullah. *Thermo-economic and environmental assessment of a combined cycle fueled by MSW and geothermal hybrid energies*. Pages 260-270.

The hybrid renewable energy-based power generation systems offer a reliable solution to mitigate the drawbacks of individual energy source. In this respect the biomass and geothermal energies have some well-known advantages (such as continuous provision) over the solar and wind energies. In the present paper, two integration modes are proposed for hybridization of geothermal heat with a biomass-driven gas turbine based combined power cycle. The Mode 1 configuration employs geothermal heat to increase the temperature of feedwater before the deaerator, whereas the Mode 2 structure applies the geothermal energy to generate more steam for the low pressure steam turbine. Detailed exergetic, environmental and economic appraisals are carried out to examine the hybrid systems performances. In order to represent an accurate comparison of the suggested hybridization modes, the systems are optimized to achieve minimum levelized electricity cost. The results have indicated better performance for Mode 2 hybridization scenario over the Mode 1. The former system yields 10.0% greater exergy efficiency with 20.1% less electricity cost compared to Mode 1, while it can generate 22.5% more electricity. Also, it brings about 22.5% lower CO2 emission. However, the Mode 2 configuration possess one drawback compared to Mode 1, which is its higher overall system cost rate by 17.9%. The results show that, the higher cost rate of Mode 2 configuration is mainly due to larger pressure ratio of the air compressor which causes more costs for the compressor and gas turbine components.

- **Keywords:** Hybrid energy; Gasification; Biomass; Thermoeconomic; Exergy analysis; Geothermal energy

Sun Yi, Azher M. Abed, Ahmed Deifalla, M. Riaz, Theyab R. Alsenani, Samia Elattar, Chun Yulei, Saleh Al Sulaie. *Exergoeconomic evaluation of a novel multigeneration process using solar driven Kalina cycle integrated with gas turbine cycle, double-effect absorption chiller, and liquefied natural gas cold energy recovery*. Pages 271-291.

This study is motivated to propose, evaluate, and optimize a solar-based multigeneration system relying on consecutive heat integration. Here, a heliostat field is configured to collect solar power and supply high-temperature air toward a nitrogen-based Brayton cycle. Afterward, the output hot air is subjected to a Kalina cycle suitable for medium-temperature heat resumption. A double-effect absorption refrigeration cycle boosted by a Liquid-based natural gas cold energy recovery unit for power generation and natural gas regasification are the other subsystems. The principal purpose is to protect the energy level of the fluid evacuating the solar field and to minimize the irreversibility of the scheme since solar-based systems lead to major irreversibility. The designed process is apprised from a 3E perspective, including exergy, energy, and exergoeconomic analyses. In addition, a comprehensive sensitivity study is done based on the influence of effective factors on the exergy and energy efficiencies and unit cost of products. Eventually, a multi-objective optimization is performed to set the most suitable condition of decision parameters and reach the optimal unit cost of products and exergy performance (objective functions). To do optimization, a genetic algorithm is applied, and two decision-making approaches, i.e., LINMAP and TOPSIS, are regarded. The optimal objectives are gauged to be 24.76% and 15.90 $/GJ by TOPSIS and 24.47% and 15.73 $/GJ by LINMAP, respectively.

- **Keywords:** Solar energy; Multi-generation; Nitrogen-based Bryton cycle; Liquefied natural gas; 3E analysis; Multi-objective optimization

Balamurugan Karuppaiah, Jeyaraman Anupriya, Shen Ming Chen, Sung Jea Park. *An emergent electrochemical sensor based on spinel zinc manganese oxide decorated on amine-functionalized boron nitride for enhanced electrochemical determination of herbicide mesotrione*. Pages 292-303.

Mesotrione (MTO) is a herbicide that is commonly used in agriculture; unfortunately, this chemical often makes its way into aqueous environments. In this study, an MTO sensor was fabricated based on spinel zinc manganese oxide (ZnMn2O4, ZMO) nanoparticles (NPs) and an amine-functionalized boron nitride (NH2-BN) composite. ZMO was synthesized using a coprecipitation technique, and NH2-BN was prepared by a urea-assisted ultrasonication/stirring method. The nanocomposite of ZMO NPs/NH2-BN was prepared using the sonication method. The crystallinity, oxidation states, and functionality of the catalysts were investigated using physiochemical characterization techniques: powder X-ray diffraction analysis, Fourier-transform infrared spectroscopy, and X-ray photoelectron spectroscopy. In addition, the surface morphology and topology of the ZMO NPs/NH2-BN composite were analyzed by field-emission scanning electron microscopy and high-resolution transmission electron microscopy. The ZMO NPs/NH2-BN/glassy carbon electrode (GCE) exhibited a well-resolved MTO reduction peak in cyclic voltammetry experiments due to the synergetic effect between the aggregated ZMO NPs and NH2-BN. In addition, ZMO NPs/NH2-BN/GCE exhibited a low limit of detection of 1.5 nM, high sensitivity (1.791 μA μM−1 cm−2), and broad linear ranges (0.01–12.51 μM and 18.51–1777.51 μM). A ZMO NPs/NH2-BN/GCE sensor prototype was used to effectively detect MTO in environmental water samples with good recovery.

- **Keywords:** BN; Amine functionalization; ZnMn2O4; Electrochemical sensor; Herbicide mesotrione; Real sample analysis

Shichao Wu, Tichang Sun, Jue Kou, Enxia Gao. *Green and efficient separation of iron and phosphorus from high-phosphorus oolitic iron ore by reduction roasting without a dephosphorization agent*. Pages 304-315.

To provide a new method for the dephosphorization of high-phosphorus oolitic iron ore (HPOIO) by reduction roasting, the feasibility of the high-efficiency separation of iron and phosphorus by reduction roasting and magnetic separation process (RRMSP) without a dephosphorization agent was studied. The results showed that the full separation of iron and phosphorus was achieved without a dephosphorization agent. Under optimal conditions, powdery reduced iron (PRI) with 92.77% iron and 0.09% phosphorus content was produced. Iron recovery and dephosphorization reached 68.70% and 93.50%, respectively. In a weak reducing atmosphere, apatite was not reduced. A portion of the phosphorus in the iron minerals formed apatite, and the remaining phosphorus entered fayalite. Metallic iron and phosphorus minerals were physically separated. Compared with the addition of dephosphorization agent, clean production was realized without the addition of dephosphorization agent, but the iron recovery was not ideal; the economic benefits should be further studied in the future.

- **Keywords:** High-phosphorus oolitic iron ore; Separation of iron and phosphorus; Reduction roasting; Without a dephosphorization agent

Moein Besharati Fard, Abolfazl Hamedani, Mehdi Ebadi, Donya Hamidi, Kasra Motlaghzadeh, Mohammadreza Emarati, Di Wu, Gordon Mckay. *Sustainable waste-to-energy plant site selection by a hybrid method of geographic information system and evidential reasoning: A case study Guilan province*. Pages 316-331.

A new hybrid method of utilizing Evidential Reasoning (ER) approach and Geographic Information System (GIS) was applied to find the optimum location of a Combined Heat and Power (CHP) incineration plant in Guilan province. According to guidelines and prevailing conditions, thirteen criteria were analyzed and divided to three main sections of environmental, social and economic categories. Most of the data in the study were obtained from local organizations and satellite images. To weight the criteria, evidential reasoning was applied to aggregate the decision-makers' opinions, and to find the potential sites; spatial analysis was done through the GIS. The result of suitability analysis indicates that about 0.07 % of total area of Guilan province is "the most suitable" region for the incineration plant and 0.05 %, 0.07 %, 2.77%, and 97.04 % are in the class of "suitable", "relatively suitable", "least suitable" and "limited". The areas with an area of larger than 40,000 m2 which is the necessary area for a 9 MW incineration plant were classified as alternatives for incineration CHP plant locations (A1-A7). All the locations were investigated to be near rural areas, which might bring inevitable harm to the adjacent communities. Also, the low amount of "most suitable region" and "suitable region" foster a sense of concerns, which should be addressed by applying a sustainable approach for preserving the environment. The techno-economic analysis presented in this study indicates that the project is not economically beneficial at all.

- **Keywords:** Multi-criteria decision-making; Evidential reasoning; Incineration CHP plant; Geographical information system; Site selection

Kamal Benali, Rachid Benhida, Khaoula Khaless. *A novel and complete process for iodine extraction and recovery from industrial wet-process phosphoric acid based on chemical oxidation and solvent extraction*. Pages 332-345.

Due to their copious availability and broad applicability, iodine recovery from numerous sources, such as byproducts of various industrial processes, has attracted attention. To meet growing market demand for iodine as well as to accomplish long-term management of iodine resources, phosphate rocks and their derivatives were discovered as a possible source of iodine. As phosphoric acid is produced in significant quantities each year more than 20 million tons the extraction of iodine, a byproduct of the wet processing of phosphoric acid, is crucial. This research aims to develop a pre-oxidation and solvent extraction-based method for recovering high purity iodine from wet phosphoric acid (SX). For this purpose, the effects of operating variables, such as: time, acidity, dose of the oxidant, temperature, volume ratio, and the concentration of stripping solution have been studied. Using 30% H2O2 as an oxidant, all the iodides ions present in wet phosphoric acid was converted into elemental iodine. The iodine was then extracted and stripped quantitatively using pure kerosene and 0.02 M sodium sulfite at ratios (O:A) of 1:2 and 1:1, respectively. The resulting iodine precipitate was subjected to several analyses, including iodometric titration, XRD, and ICP-OES, which confirmed its purity to be 99.9%. Finally, a flowchart process for both recovering and reducing the loss of iodine from wet phosphoric acid was developed without interfering with the normal fertilizer production route.

- **Keywords:** Iodine; Wet-phosphoric acid; Extraction; Pre-oxidation; Solvent extraction

Hongsheng Ma, Zhiyu Liu, Yang Li, Jiaqing Zhang, Yubiao Huang, Changjian Wang. *Effects of ignition energy, oil volume and ignition position on transformer oil explosions*. Pages 346-356.

The transformer oil is easy to explode in enclosed power equipment. However, the explosion characteristics of transformer oil have not been clearly clarified in previous studies. In this paper, the effects of ignition energy, oil volume, and ignition position on the overpressure buildup and fireball behavior caused by transformer oil explosions are investigated. Experimental results show that four typical stages of cloud occlusion, rapid development, combustion stage and free diffusion can be found during the fireball evolution. The fireball shape is significantly affected by the ignition position. With the increase of oil volume, both the maximum fireball radius and the maximum fireball area gradually increase. The double-peak overpressure structure is first observed and the first peak overpressure is always larger than the second one. The first overpressure peak is generated by the explosive explosion while the second overpressure peak is induced by the coupling between the combustion waves of initial fireballs and the reflected waves of shock waves induced by the explosive. With the increase of oil volume, the maximum overpressure decreases due to the energy absorption. The maximum overpressure for center ignition is larger than that for bottom ignition or top ignition.

- **Keywords:** Transformer oil explosion; Fireball area; Explosion overpressure; Oil-gas mixture

Xi Chen, Ibrahim B. Mansir, Bhupendra Singh Chauhan, Saleh Mahmoud, Hamdi Ayed, Hassen Loukil, Ruicheng Tian, Wael Al-Kouz. *Proposal of a biogas upgrading process for a novel eco-friendly trigeneration model, producing power, methanol, and desalinated water*. Pages 357-374.

Non-renewability and difficult access to fossil fuels can be replaced with renewable fuels, such as biogas. Due to the close structure of biogas to fossil fuels, it has become a powerful fuel for energy systems, especially when it enters the upgrading process. With this in mind, the proposed system proposes a novel trigeneration model integrated into a biogas upgrading unit, producing electricity, desalinated water, and methanol. This process is proposed for the first time, which is able to increase the thermodynamic, economic, and environmental performances compared to previous studies. Negative CO2 emission is its main feature that is available using a methanol synthesis unit. Thermal desalination and ammonia Rankine cycles are other equipment used in the proposed structure. The whole system is simulated in the Aspen HYSYS software and is investigated from the 4E aspect, namely energy, exergy, economics, and environment. Also, a sensitivity study is conducted. The overall energy and exergy efficiencies equal 51.54% and 87.39%, respectively. These criteria are improved between 4.54% and 15.64%-points and 32.29–74.70%-point compared to the existing literature review, respectively. In addition, the net CO2 emission intensity equals −0.54 kgCO2/kgMeOH, which is considerably lower than other relevant technologies (between 1.78 and 10.68 times). Moreover, the unit cost of methanol in the proposed process equals 0.21 $/kg, which is 63.54–85.61% lower than other methods available in the literature review.

- **Keywords:** Biogas upgrading; Methanol; Desalination; Thermodynamic analysis; Economic analysis; Negative carbon dioxide emissions

Sonia Arriaga, Maria Federica Carboni, Piet N.L. Lens. *Effect of static magnetic field exposure on biohydrogen production via dark fermentation of glucose*. Pages 375-388.

The effect of a static magnetic field (SMF) on the microbial activity of anaerobic granular sludge was investigated using a SMF field provided by a magnetic platform with

intensities between 30 and 90 mT. BioH2 production was assessed in fed batch fermentation tests from glucose using anaerobic granular sludge with (HT) and without (WHT) heat shock pretreatment (100 ºC, 1 h). Under the conditions tested, 70 mT SMF was the best condition for bioH2 production, with a threefold decrease of lag time, a 12–50% increase in bioH2 production rate, and an improved consumption of iron and phosphate, compared to the controls (no SMF). Exposure to the SMF induced modifications in volatile fatty acid (VFA) production, pH and conductivity, biomass concentration, exopolysaccharide (EPS) composition as well as size and settleability of the granular anaerobic sludge. Microbial analysis showed that in the presence of the SMF, the relative abundance (RA) of Clostridium and Lactobacillus increased in both HT and WHT sludges, while it decreased the RA of Methanosaeta and Methanobacterium. The RA of Terrisporobacter increased with the heat shock, and also the stimulation along the fed batch cycles improved the RA of Terrisporobacter with and without SMF. The application of the SMF as a pre-treatment of inoculum and during bioH2 production seems to be an interesting and easy scaling up strategy to shorten the start-up of the dark fermentation process and help reducing the microbial diversity of the sludge, favouring more specialized species for bioH2 production.

- **Keywords:** Static magnetic field; Biohydrogen; Glucose; Lag times; EPS; Settleability

Peiliang Sun, Xiangdong Li, Xingxing Cheng, Zhiqiang Wang, Peng Wang. *Transition metal modified Mn-based catalysts for CO-SCR in the presence of excess oxygen*. Pages 389-401.

The CO-SCR technology based on transition metal is of great significance for NOx removal in large-scale industrial production. However, excess oxygen usually hinders the deNOx reaction in the actual industrial process. In this paper, a series of Mn-based catalysts modified by transition metals (Fe, Ni, Cu) were prepared using the co-precipitation method, which aimed to obtain good CO-SCR performance under O2-rich condition. The results showed that the Cu-Mn2 sample exhibited excellent deNOx performance. Regardless of the presence or absence of oxygen, the NO conversion of Cu-Mn2 catalyst was remain about 60% and 95% at 350 and 400 ℃, respectively. Differently, the NO conversion of Fe-Mn2 catalyst significantly increased from approximately 10% to 61% at 400 ℃ after introducing oxygen, which proved that excess oxygen could promote the CO-SCR process over Fe-Mn2 sample. The varied physical and chemical properties of the prepared materials were thoroughly evaluated through BET, SEM, XRD, XPS and in situ DRIFTS technologies. The results demonstrated that perovskite α-Mn2O3, decahedral Mn5O8, Fe2O3 and Fe3O4 crystals were the dominant structures promoting deNOx reaction on the Fe-Mn2 catalyst. The oxidation of low valence nitrogen oxides by decahedral Mn5O8 on Fe-Mn2 catalyst was an important factor for oxygen resistance. And the various spinel structures over Ni-Mn2, and Cu-Mn2 indicated strong synergistic effects. For the Cu-Mn2 catalyst, the strong synergistic effect of Cu-□-Mn species could promote the dissociation of intermediate -NONO. O2 tended to occupy the surface synergetic oxygen vacancies in Cu-□-Mn species at high temperatures, which could inhibit the dissociation of -NONO and enhance the CO oxidation reaction. The possible reaction mechanisms for CO-SCR over Mn-based catalysts were discussed specifically.

- **Keywords:** Transition metal; Mn-based catalyst; CO-SCR; Multivalent catalysis; Surface synergetic oxygen vacancy

Po Li, Xiang Li, Hao Wang, Feng Guo. *A comparative experimental study on emission characteristics and ammonia energy ratio of diesel generator operating in ammonia/diesel dual fuel mode by premixed and port injection*. Pages 402-410.

The extensive use of traditional fossil fuels has exacerbated crises such as environmental pollution, depletion of non renewable energy and global greenhouse effect. Ammonia (NH3) is considered a promising fuel to replace conventional fossil energy in internal combustion engines. A four-cylinder, four-stroke commercial diesel generator (HTD-20GF) was modified and two different ammonia fuel injection systems, premixed charge compression ignition (PCCI) combustion and gas phase port injection (GPPI), were developed. The exhaust emission characteristics, thermal efficiency and ammonia energy ratio of ammonia/diesel dual fuel (ADDF) generator in both PCCI and GPPI modes were studied. The experimental results showed that the overall NO emission in GPPI mode was lower than that in PCCI mode. From the experimental results, both PCCI and GPPI mode can reduce CO2 emission. The GPPI mode was significantly more effective than the PCCI mode in reducing the volume fraction of CO2 in the exhaust gas. Compared with all diesel mode, the HC content in the exhaust gas got worse at lower ammonia energy ratio in both modes, but the increase rate of HC emissions slightly improved as the ammonia energy ratio increased. However, PCCI and GPPI modes reduced the thermal efficiency of the generator, and ammonia had a more negative effect on the thermal efficiency of the ADDF generator in PCCI mode.The experimental results also tested the limiting ammonia energy ratio of this commercial generator at 1 kW. In summary, this study provides a new perspective on the different feeding methods of ammonia as a fuel, which may contribute to the selection of fuel injection methods for ammonia engines to decrease emissions.

- **Keywords:** Ammonia/diesel dual fuel generator; PCCI; GPPI; Ammonia energy ratio; Exhaust emissions; Thermal efficiency

Mingqi Bai, Meng Qi, Chi-Min Shu, Genserik Reniers, Faisal Khan, Chao Chen, Yi Liu. *Why do major chemical accidents still happen in China: Analysis from a process safety management perspective*. Pages 411-420.

As an important consideration in the chemical industry, chemical process safety has received notable attention in China. However, catastrophic chemical accidents still occur. To better understand why accidents continue to occur, this paper presented a diagnostic analysis of 14 major chemical accidents in China from 2012 to 2022 based on VOSviewer software. The authors analysed the correlation between the accident causation and their relationship with the safety management elements. The study observed that inferior process safety culture, intentional violation (rule-breaking) of procedure, inadequate safety training, and illegal operations were the most frequent causes of accidents. These causes highlighted the prominent gaps in PSM in China in the process safety culture, compliance with standards, the conduct of operations, process safety competency, and training & performance assurance. The results based on co-occurrence analysis indicated a strong correlation between these gaps in PSM. Enterprises should pay attention to collaborative management among them. These deficiencies in the enterprise's PSM system showed that the essential defects in China's chemical industry are a poor safety culture, inadequate accident investigation, inadequate training, and a lack of chemical safety personnel. The study recommended that the chemical industry establish superior process safety culture and competency for all personnel, monitor leading and lagging process safety indicators, apply inherent safety, and practice advanced safety management concepts. We hope that the findings can provide China's perspectives and strengths for global chemical safety.

- **Keywords:** Chemical process safety; Accident causation; Safety management elements; Process safety culture; Accident investigation

Peng Cheng, Cong Yang, Shang Zhou, Junyu Huang, Rongrong Liu, Bing Yan. *Degradation efficiency of antibiotics by the sewage-fed microbial fuel cells depends on gram-staining property of exoelectrogens*. Pages 421-429.

Microbial fuel cells (MFCs) are green technologies for bioenergy capture. Gram-negative bacteria have been shown as the dominant electrogenic functional microbes on the anode of MFC. However, how gram-positive bacteria perform in the mixed colonies remains unclear. In this study, specific classes of antibiotics are employed to characterize the properties of electroactive microorganisms in the sewage-fed MFC. Our results reveal that MFCs exhibit high efficiencies in degrading some widely used bacterial antibiotics and generating electricity, while being significantly influenced by gram-staining properties of microbial communities. The MFC is effective against the broad-spectrum bacterial antibiotic cefepime with a degradation efficiency of 92.5% (5 mg/L) and a maximum power density of 263.6 mW/cm2 (25 mg/L). Electrochemical analyses demonstrate that the gram-positive bacteria on anode are more resistant to their specific antibiotic vancomycin and the maximum power output of the system is enhanced by 13.7%. Furthermore, the exoelectrogens in the mixed colonies show insensitivity to fungi-specific antibiotics such as amphotericin with extremely low degradation rate (<4.5%). Our findings provide a new perspective on exploring the characteristics of functional exoelectrogens based on the microbial responses to antibiotics with specific antibacterial spectrum. It is also crucial to guide the application of bioelectrochemical systems in medical wastewater treatment for urban sustainable development.

- **Keywords:** Microbial fuel cell; Exoelectrogens; Antibiotics; Gram staining

Shuda Hu, Shihang Li, Hui Cheng, Hao Jin, Jun Hou, Changgeng Gui, Xingyue Chen, Liang Yuan, Fubao Zhou. *Study on the wet dust collection mechanism of metal-based filter screens and the effect of its inclination angle on dust removal performance.* Pages 430-437.

The wet filter dust collector (WFDC) is widely used in dust control in various industries, but its dust collection mechanism is unclear, and the influence of the metal-based filter screen (MBFS) inclination angle on the dust removal performance is still uncertain. In this paper, the liquid film crushing and collecting dust mechanism of MBFS and the influence of its inclination angle on the dust removal performance of WFDC are studied. The results show that with the increase of inclination angle (30° to 150°), the average pressure drop of WFDC first decreases and then increases, the average dust concentration first increases and then decreases, and the MBFS dust removal performance is optimal at 90°. The optimized WFDC was applied on-site in a coal preparation plant, which exceeded the dust suppression efficiencies of 91 % and 88 % for total dust and respirable dust, respectively. The research results are expected to provide theoretical guidance for WFDC design and improvement.

- **Keywords:** Wet filter dust collector; Metal-based filter screen; Inclination angle; Dust control; Performance evaluation model

Wenchang Wu, Menghui Zhang, Liang Zhao, Hui Dong, Jiyu Zhang. *CFD-DPM data-driven GWO-SVR for fast prediction of nitrate decomposition in blast furnaces with nozzle arrangement optimization*. Pages 438-449.

In the industrial production process, it is important to improve the productivity of blast furnaces in response to the worldwide call for energy saving and emission reduction. In

this study, a data-driven method using computational fluid dynamics (CFD) is developed for the rapid prediction of nitrate decomposition in a blast furnace. The method includes the creation of a CFD database, for which nozzle arrangement patterns, relative distances, spray cone angles and temperatures are simulated and collected. Support vector regression (SVR) hyperparameters are optimized using genetic algorithm (GA), particle swarm optimization (PSO), and gray wolf optimizer (GWO). Machine learning interpretability methods shapley additive explanations (SHAP) and partial dependence plots (PDP) are used to analyze the impact of features on prediction results. The results show that the hybrid GWO-SVR model has a better performance, with the degree of fit (R2) improving from 0.7752 to 0.9719. When the distance is taken around 0.58, increasing the temperature and cone angle is more favorable to improve the decomposition rate of the blast furnace. SHAP method shows that only the arrangement 2 and 4 have a positive effect on improving the decomposition rate. The response time for accurate prediction of nitrate decomposition rate is 259200 times shorter than that of industrial-scale CFD simulations. The method is also used to determine the best combination of solutions. This cross-disciplinary approach provides a time-saving and cost-effective tool for improving the response of blast furnace productivity to changes in nozzle arrangement.

- **Keywords:** Computational fluid dynamics; Thermal decomposition reaction; Blast furnace; Machine learning algorithms

Tongsheng Zhang, Hui Peng, Chang Wu, Yiqun Guo, Jiawei Wang, Xinzhi Chen, Jiangxiong Wei, Qijun Yu. *Process compatible desulfurization of new suspension preheater cement production: Rapid catalytic oxidation of trace SO2 over V2O5-based catalysts in preheater environment*. Pages 450-461.

Efficient capture of sulfur dioxide (SO2) in the preheater of the cement production system is the key to achieving process compatible flue gas desulfurization (FGD). Herein, the rapid oxidation of trace SO2 over V2O5-based catalysts in the preheater environment was realized to enhance the SO2 capture capacity of limestone in raw meal, and the catalytic efficiency was further improved by 45.2%, 56.1% and 61.9% after introducing TiO2/MnO2/CeO2 as cocatalysts, respectively. The V2O5-based catalysts had superior catalytic behavior only when the flue gas temperature exceeded 500 °C, while the composition variation of flue gas had a minor influence on SO2 oxidation. Finally, a maximum SO2 oxidation efficiency of 68.1% was achieved in the presence of 4.0% O2, 25.0% CO2 and 15.0% H2O at 600 °C. Furthermore, the mechanism of SO2 catalytic oxidation over V2O5-based catalysts was deduced based on the results of XRD, BET, XPS and Raman, and V5+ was identified as the primary vanadium species for SO2 oxidation. The results provide a deeper insight into the catalytic oxidation of SO2 in the preheater environment, and then facilitate the improvement of process compatible FGD and available dry FGD technologies for cement industry.

- **Keywords:** SO2; Catalytic oxidation; Flue gas desulfurization; V2O5-based catalysts; Preheater environment

Tianru Li, Baomin Wang, Xiong Zhang, Xiao Han, Yunqing Xing, Chengcheng Fan, Ze Liu. *Effect of nano silica on solidification/stabilization of heavy metal in alkali-activated MSWI fly ash solidified body*. Pages 462-474.

Municipal solid waste incineration fly ash (MSWIFA) containing considerable heavy metals is classified as a hazardous waste. Alkali-activated technology can effectively improve the environmental safety of MSWIFA. Due to the low silica content of MSWIFA, the addition of nano silica (NS) solves the problem to enhance the ability of solidification/stabilization

(S/S) and maximize the utilization of MSWIFA. NS/MSWIFA solidified body was prepared by alkali-activated technology in this work. The mechanical and environmental properties of NS/MSWIFA solidified body with various dosages (0–3 wt%). NS were characterized by compressive strength, leaching concentration, and chemical speciation distribution of heavy metals. A comparative study of MSWIFA and solidified bodies for exploring S/S mechanisms was investigated using XRD, FTIR, TG/DTG, NMR, and SEM/EDS tests. The results showed that the leaching concentration of Pb in MSWIFA based on different leaching methods was 23.54 mg/L and 31.7 mg/L, 19.6 times higher than the standard of hazardous waste landfill and 126.8 times higher than the standard of landfill site of municipal solid waste, respectively. The total amount of Zn and Pb was 4739 mg/kg and 2451 mg/kg, respectively, exceeding other heavy metals by 1–2 orders of magnitude. When the addition of NS was 2 wt% and 3 wt%, the compressive strength and the leaching concentration of heavy metals in solidified bodies reached the highest and the lowest, respectively. Comparative analysis indicated that adding NS promoted heavy metals in MSWIFA to be converted into a stable state, and increased hydration product C-(A)-S-H gels formation, making the structure denser. On a broader perspective, NS/MSWIFA solidified body was developed as a low-carbon and environment-friendly binder.

- **Keywords:** Solidification/stabilization; MSWI fly ash; Nano silica; Alkali-activated technology; Heavy metal

Parth Patel, Til Baalisampang, Ehsan Arzaghi, Vikram Garaniya, Rouzbeh Abbassi, Fatemeh Salehi. *Computational analysis of the hydrogen dispersion in semi-confined spaces*. Pages 475-488.

Although green hydrogen is an appropriate clean energy alternative, hydrogen leakage and dispersion are the challenges to establishing safe and reliable hydrogen infrastructure. Released hydrogen in confined or semi-confined space may build up flammable gas clouds, which can have severe consequences for the safety of human life and property. Proper ventilation systems will help in reducing hydrogen gas accumulation. This study presents a comprehensive study to analyse hydrogen dispersion behaviour and the influence of ventilation variations on hydrogen volumetric concentration and stratification. A computational model is developed for the leakage diffusion of hydrogen in an enclosed cuboid space with roof and door ventilation. A detailed analysis is conducted to shed light on the impact of door and roof ventilation positions on forming the flammable cloud. It is observed that the displacement flow and multi-layer stratification are established in the absence of wind or imperceptible air circulation. Single-vent configurations were ineffective, when installed at the top of the leakage point, but multiple-vent arrangements incorporating door and roof vents were found to be more efficient in extracting hydrogen. However, it should be noted that not all multiple-vent arrangements may meet safety requirements. The result indicated that the optimal arrangement for minimizing the size of a flammable cloud involves placing the door vent close to the ceiling while situating the roof vent near the source of leakage. These findings will aid in devising strategies for minimizing the occurrence of flammable cloud formation and preventing hydrogen fire and explosion incidents within partially enclosed facilities.

- **Keywords:** Hydrogen safety; Computational fluid dynamics (CFD); Low-velocity hydrogen leakage; Ventilation

Uyen Dao, Rioshar Yarveisy, Shams Anwar, Faisal Khan, Yahui Zhang, Hai H. Ngo. *A Bayesian approach to assess under-deposit corrosion in oil and gas pipelines*. Pages 489-505.

Under-deposit corrosion (UDC) and microbiologically influenced corrosion under deposits (UD-MIC) have increasingly been identified as severe forms of localized corrosion

threatening the integrity of pipelines. This work utilizes a knowledge-based, semi-quantitative Bayesian approach to capture UDC and UD-MIC susceptibility and severity. This article proposed a Bayesian Network framework to study susceptibility to UDC and UDC corrosion rate. The effective corrosion rate is introduced as a measure to combine the susceptibility and corrosion rate. This measure could identify high-risk locations by assessing the probable corrosion rate while highlighting the pipeline's vulnerability to deposit settlement. Four case studies of pipeline failures due to UDC illustrate the framework's validity. A case study for a sweet gas pipeline is adapted to explore the model's robustness in assessing cases with low probabilities of UDC occurrence. The gas pipeline data, the corrosion key performance indicators spanning six years, general information on the pipeline, and the Bayesian network are made publicly available through a repository.

- **Keywords:** Under deposit corrosion; MIC; Bayesian method; Bayesian network; Pipeline

Jian Tang, Jiabin Zhuang, Loai Aljerf, Heng Xia, Tianzheng Wang, Bingyin Gao. *Numerical simulation modelling on whole municipal solid waste incineration process by coupling multiple software for the analysis of grate speed and air volume ratio*. Pages 506-527.

Uncertainties in the calorific value and composition of municipal solid waste (MSW), the variability in operations, equipment performance decline, maintenance needs, and other dynamic factors make it challenging for operational experts to accurately gauge the overall combustion impact under fluctuating conditions. There is a need for a visual numerical simulation of the full MSW incineration (MSWI) process, with a focus on the effectiveness of the grate speed and air volume ratio. Unfortunately, software like Aspen Plus struggles to visually depict the effect of typically manipulated variables such as grate speed, and it is not well-suited for simulating solid-phase combustion and flue gas treatment. In response to these challenges, our study introduces a numerical simulation method for the MSWI process using a multi-software coupling approach. This simulation method incorporates (a) the use of custom software for simulating solid-phase combustion on the grate, (b) the application of Computational Fluid Dynamics (CFD) software for gas-phase combustion in the furnace, and (c) the utilization of chemical process simulation software for non-grate solid-phase combustion. The benchmark condition was determined using real-time running data from the Beijing MSWI Power Plant. The results show that for the incinerator’s third flue, flue gas G1, and flue gas G3, the relative errors between the simulated and actual values for flue gas temperature and oxygen concentration were 0.3% and 1.1%, 3.5% and 20%, and 0.2% and 20% respectively. In addition, we used eight non-benchmark conditions to study the effects of grate speed and air volume ratio. When the grate speed was gradually increased from 6 m/h to 8 m/h, O2, CO2, sulfur dioxide (SO2), sulfur trioxide(SO3), nitrogen monoxide (NO), and nitrogen oxide (NO2) at G1 had error fluctuation ranges of 5.9%− 48.5%, 2.5%− 11.5%, 10.42–28.57%, 7–23%, 29.10–45.52%, and 24.39–48.78%, respectively. When the primary air ratio was gradually increased from 0.84 to 0.96, the O2 concentration at G1 exhibited a steady upward trend. The simulation results provide insights into the adjustment range of the manipulated variables and offer additional support for the visualized and optimized control operation of the MSWI plant.

- **Keywords:** Municipal solid waste incineration (MSWI); Numerical simulation; Multiple software coupling; Grate speed; Air volume ratio; Control optimization

Haihang Li, Zhenlin Li, Qiang Wang, Yajun Huang, Fei Tang. *Heat transfer and spread characteristics of continuous ethanol spill fires on sand substrates*. Pages 528-536.

Spill fire is common in industry, with the characteristics of large burning area and difficult to extinguish. To study its mechanism more deeply, a series of experiments of ethanol spill fire were carried out on sand substrate. The flame spread distance was measured, and the heat feedback and burning rate were analyzed. The experimental results showed that 0.25 mm sand made the proportion of heat conduction feedback in the quasi-steady stage reach about 70% of all thermal heat feedback, and the steady burning rate also reached the maximum value. With the increase of sand size, the proportion of heat conduction feedback decreased, the heat convection feedback gradually dominated, and ultimately the steady burning rate decreased first and then increased. This showed that sand affected the heat transfer in the quasi-steady stage of spill fire by changing the heat transfer process and the proportion of three modes of heat transfer, thus changed the steady burning rate. Furthermore, the influence of sand on the spread of ethanol in terms of mass transfer was also analyzed. For the initial spread stage, the obstructive effect of sand on the fuel spread was quantified based on Darcy's law. It was found that the obstructive capacity of sand on fuel spread had a quadratic relationship with its specific surface area.

- **Keywords:** Spill fire; Flame spread; Heat transfer; Burning rate; Sand substrate; Pool fire

Amirreza Javaherian, Nima Ghasemzadeh, Nima Javanshir, Mortaza Yari, Mohammad Vajdi, Hossein Nami. *Techno-environmental assessment and machine learning-based optimization of a novel dual-source multi-generation energy system*. Pages 537-559.

The utilization of high-temperature hybrid energy systems has a vital and promising role in reducing environmental pollutants and coping with climate change. So, in the present research, a dual-source multigeneration energy system composed of a gas turbine, a supercritical carbon dioxide recompression Brayton cycle, an organic Rankine cycle, an absorption refrigeration system, and a reverse osmosis desalination unit is designed and analyzed from thermodynamic, environmental and economic perspectives. The system supplies power with a stable load to follow the changes in the demand side which is important for off-grid distributed energy systems. The dual-source operation of the system makes it possible to generate sustainable electricity leading to less utilization of fossil fuels in the gas turbine subsystem and reduction in environmental pollution, and furthermore, malfunctioning of a subsystem will not lead to the failure of the entire plant. Three multi-objective optimizations with different objective functions are accomplished using artificial neural network from data learning and genetic and Greywolf algorithms to obtain the best-operating conditions. Under the base conditions, for the total input energy of 699 MW to the entire system, the energy and exergy efficiencies, the unit exergy cost of products, the carbon dioxide emission index, and the payback period, respectively, were found to be 45 %, 54 %, 15.3 $/GJ, 112.2 kg/MWh, and 7.2 years. The net output power of the proposed system was calculated as 288.2 MW. A sensitivity analysis revealed that with a change in the pressure ratio of the supercritical carbon dioxide cycle, the net generated power and overall efficiency take maximum values of 293.9 MW while the unit exergy cost of products and carbon dioxide emission index take minimum values of 15.3 $/GJ and 110.1 kg/MWh, respectively. Furthermore, increasing the pressure ratio of the gas turbine leads to maximum values of 45 % and 54 % in overall energy and exergy efficiencies, respectively.

- **Keywords:** Emission reduction; Multigeneration system; Gas turbine; Techno-environmental; Multi-objective optimization; Machine learning

Zhenxiang Pan, Mohan Song, Bizhen Zeng, Liguo Shen, Leihong Zhao, Hongjun Lin. *Novel cetyltrimethylammonium bromide modified mixed adsorbent for efficient treatment of dyeing and printing wastewater*. Pages 560-567.

The treatment of dyeing and printing wastewater is a formidable challenge due to its high chemical oxygen demand (COD) and chromaticity, which pose severe threats to both the environment and human health. In this study, a composite modified adsorption material was prepared based on the applicability and feasibility in practical engineering applications. A novel mixed modified adsorbent was developed by incorporating activated carbon and activated clay as the foundation materials, followed by the addition of cetyltrimethylammonium bromide (CTAB) for modification. The performance of the composite adsorbent was evaluated via adsorption experiments of bromophenol blue (BPB) solution and dyeing and printing wastewater. The results demonstrated that the mixed modified adsorbent achieved a remarkable removal rate of 99% for BPB and 99.3% for chromaticity, under the optimal adsorption conditions. Furthermore, the regeneration performance of the mixed modified adsorbent was found to be exceptional. The adsorption process of BPB by the composite adsorbent was governed by the quasi-second-order kinetic model and Freundlich isotherm model, as evidenced by adsorption kinetics and isotherm analyses. The straightforward preparation method, coupled with the superior adsorption performance, underlines the promising potential of the proposed composite adsorbent for practical applications.

- **Keywords:** Dyeing wastewater; Adsorption; Printing wastewater; Adsorption kinetics; Isothermal adsorption; Cetyltrimethylammonium bromide

Xiaomang Miao, Fahid Riaz, Badr Alotaibi, Manoj Kumar Agrawal, Mohammed Abuhussain, Theyab R. Alsenani, Mansoureh Alizadeh Balderlou, Qing Lin. *Performance enhancement of latent heat thermal energy storage system by using spiral fins in phase change material solidification process.* Pages 568-579.

Latent heat thermal energy storage systems (LHTESS) have recently gained attention due to the critical demand for clean energy production and storage. The influence of spiral fins on the performance augmentation of a vertical tube-shell LHTESS in the solidification process was studied numerically. Different formation of fins which includes the quadruple, triple, double and single fins were studied. Amount of phase change material (PCM) mass inside the PCM enclosure was preserved equal in all cases and the length of the fins were adjusted for different fin numbers to keep the surface of heat transfer constant to find the optimized fin number. The phase change process was simulated by adopting the enthalpy-porosity technique. It was observed that the triple fin case outperformed other cases and the single fin case showed the least enhancement. When comparing the different cases while the heat transfer surface was kept constant, the triple fin case shows better performance in terms of time averaged Nusselt number and total solidification time respectively. It was revealed that the performance enhancement was not directly proportional with the number of fins and there was a trade-off between fin number and length of each fin.

- **Keywords:** LHTESS; Energy Storage; Spiral Fin; PCM; Solidification; Paraffin Wax

Michelle Mei Xue Lum, Kim Hoong Ng, Sin Yuan Lai, Abdul Rahman Mohamed, Abdulkareem Ghassan Alsultan, Yun Hin Taufiq-Yap, Mei Kee Koh, Mohamad Azuwa Mohamed, Dai-Viet N. Vo, Manjulla Subramaniam, Kyle Sebastian Mulya, Nathasya Imanuella. *Sulfur dioxide catalytic reduction for environmental sustainability and circular economy: A review*. Pages 580-604.

Air pollution sourced from untreated sulfur dioxide-rich flue gas is one of the major environmental and human health issues. Throughout the years, many sulfur dioxide removal technologies have been invented and implemented on a wide scale. Despite the high sulfur dioxide removal efficiency of conventional treatment methods, such as limestone-gypsum desulfurization and spray dry absorption, they generate a large number of secondary sulfur-containing by-products. Thus, sulfur dioxide catalytic reduction, with the help of suitable reducing agents, is sustainable with acceptable desulfurizing efficiency while recovering valuable solid sulfur. Herein, we review advances in sulfur dioxide catalytic reduction with critical insights contributed by internal and external factors. Sulfur dioxide catalytic reduction is a regenerative desulfurization treatment with lower space requirement and water consumption, simultaneously transforming waste sulfur dioxide to elemental sulfur. Catalytic sulfur dioxide reduction to sulfur via transition metal-based catalysts (copper-alumina and nickel-alumina) and sulfided metal-based catalysts (cobalt-molybdenum/γ-alumina) appeared to be highly promising for complete sulfur dioxide conversion (100%) while maintaining high sulfur selectivity (more than 99.5%). High industrial and market demands for solid sulfur have also imposed great opportunities to advance this technology. However, the critical weaknesses of sulfur dioxide catalytic reduction are low process maturity and relatively energy-intensive, which is threatened by the high performance of conventional flue gas desulfurization and energy-efficient emerging desulfurization methods. Hence, several strategic directions through threat, opportunity, weakness, and strength analysis (TOWS) are discussed in-depth based on the strength, weakness, opportunity, and threats (SWOT) findings. In realizing environmental sustainability and a circular economy, sulfur dioxide catalytic reduction is a promising method to mitigate sulfur dioxide pollution while transforming waste-to-product, and this study serves as a guide to making sulfur dioxide catalytic reduction a mainstream desulfurization technology.

- **Keywords:** Sulfur dioxide reduction; Waste-to-product; Sulfur; SWOT analysis; Environmental sustainability; Circular economy

Majid Mohammadi, Mehdi Sedighi. *Optimizing the CO2 conversion for the sustainable production of light olefins using Cu-ZnO-ZrO2/SAPO-34 bifunctional catalysts*. Pages 605-617.

This study aims to optimize the operating conditions for one-step carbon dioxide hydrogenation to light olefins using ternary CuZnZr metal oxide and SAPO-34 zeolite catalysts. The catalyst was prepared using hydrothermal and co-precipitation synthesis, and it was characterized using XRD, TEM, BET, SEM, H2-TPR, and NH3-TPD techniques. The impact of temperature, space velocity, and H2/CO2 ratio on CO2 conversion, olefins selectivity, and CO selectivity was studied using response surface methodology (RSM). The desirability function was used to optimize multiple responses in the CO2 hydrogenation process at the same time. It takes into account the lower and upper limits, as well as the targets for each response, and produces a score that can be used to determine the best experimental conditions. It is possible to maximize CO2 conversion and olefin selectivity while minimizing CO selectivity by analyzing the optimal parameters. The optimal conditions were determined to be 375 °C, a space velocity of 9 L/g.h, and an H2/CO2 ratio of 3. The CO2 conversion rate was 16.56%, the olefins selectivity was 77.24%, and the CO selectivity was 67.91% under these conditions. The hybrid catalyst also demonstrated remarkable stability after 100 h of operation without

losing activity. The results of the study show that the CuZZ/SAPO-34 catalyst has the potential to effectively reduce CO2 to light olefins under optimized conditions.

- **Keywords:** Light olefins; CO2 hydrogenation; CuZZ/SAPO-34 catalyst; Temperature; Process optimization

M.J. Luján-Facundo, J.A. Mendoza-Roca, A. Bes-Piá, E. Zuriaga-Agustí, Sergio Mestre, María-Dolores Palacios. *Low-cost ceramic membranes manufacture using INKJET technology for active layer deposition and validation on membrane bioreactors.* Pages 618-626.

The fabrication of eco-friendly ceramic membranes based on low-cost raw materials, using digital INKJET printing techniques for active layer deposition and its validation in a membrane bioreactor (MBR) has been studied. The raw materials used in the manufacture of the support layer were UA50/2 clay, chamotte, calcium carbonate and potato starch. A MBR laboratory plant was operated to treat municipal wastewater with three ceramic membranes with different grammages in the selective layer deposition. The membrane performance at laboratory scale was evaluated in terms of transmembrane pressure (TMP) evolution for a constant permeate flux, permeate quality and mixed liquor characteristics. From these experiments, it was selected the membrane which obtained the lowest TMP profile maintaining appropriate water quality parameters (chemical oxygen demand (COD) removal percentage around 90% and turbidity around 0.06 NTU). This membrane was also operated at pilot plant scale in order to validate it at higher scale. Results indicated that TMP values were in the range of 0.06 and 0.1 bar, COD removal percentage was around 98% and microbiology analysis demonstrated that the quality of the effluent, according to European regulation 2020/741, can be classified as Class A and it can be reused for non-potable purposes.

- **Keywords:** Membrane bioreactor; Low-cost ceramic membranes; Transmembrane pressure; Laboratory plant; Pilot plant

Yang Bu, Yichun Wu, Xianlong Li, Yiru Pei. *Operational risk analysis of a containerized lithium-ion battery energy storage system based on STPA and fuzzy evaluation.* Pages 627-640.

Lithium-ion battery energy storage system (BESS) has rapidly developed and widely applied due to its high energy density and high flexibility. However, the frequent occurrence of fire and explosion accidents has raised significant concerns about the safety of these systems. To evaluate the safety of such systems scientifically and comprehensively, this work focuses on a MW-level containerized lithium-ion BESS with the system-theoretic process analysis (STPA) method. The work identified 53 unsafe control actions and corresponding loss scenarios. By combining loss scenarios and expert evaluation opinions, the key risk factors for system operation are obtained. Finally, this work proposed corresponding countermeasures and suggestions to address the key risk factors and improve the safety and reliability of the entire system operation. This work discusses the operational risks of MW-class containerized lithium-ion BESS and provides technical guidance for engineers in system designs, safe operations, and engineering applications.

- **Keywords:** Lithium-ion Battery; Containerized Energy Storage System; System-Theoretic Process Analysis; Expert Evaluation

Shannan Xu, Jingwen Yang, Fatma Marrakchi, Manman Wei, Yong Liu, Yayuan Xiao, Chunhou Li, Shuang Wang. *Macro- and micro-algae-based carbon composite for pharmaceutical wastewater treatment: Batch adsorption and mechanism study*. Pages 641-652.

Biochar synthesized from algal biomasses acts as an efficient adsorbent to remove tetracycline (TC) from aqueous solutions. In this study, a mixture of Enteromorpha (EN) and Chlorella vulgaris (CV) was pyrolyzed at 500 °C, then activated with NaOH at 800 °C to prepare composite biochar (ECA-B). The effects of TC concentration (50–500 mg·L−1), pH (3–11), temperature (30 °C–50 °C), and contact time (0–960 min) on TC absorption were investigated. Results revealed that in aqueous solutions, the biochar (EC4:1-0.5)prepared with CV and EN at the mass ratio of 4:1 and the impregnation ratio of 0.5 had the optimal TC adsorption capacity (Qm = 376.878 mg·g−1). The removal rate of EC4:1-0.5 remained above 80 % after five cycles. The surface area of EC4:1-0.5 (583.329 m2·g−1) increased by three and four times that of EN and CV, respectively. Intraparticle diffusion was considered as the major limitation for the adsorption of TC onto EC4:1-0.5. This investigation provides a method for the synthesis and optimization of algal biomass-based activated carbon for the absorption of organic pollutants in wastewater.

- **Keywords:** Tetracycline; Biochar; Algal biomass; Adsorption capacity; Surface area; Composite activated carbon

Yangwei Wu, Aijun Li, Su Lei, Tong Zhang, Qian Deng, Haoyu Tang, Hong Yao. Prediction of pyrolysis product yield of medical waste based on BP neural network. Pages 653-661.

Predicting pyrolysis product yields becomes more and more important for the realization of harmless, reduction, and resource disposal of medical waste. Based on the gray correlation analysis, this study predicted the three-state yield of medical waste pyrolysis products by building a BP neural network model. A database of pyrolysis product yields distribution of multivariate organic solid waste was established by selecting 225 sets of literature data in the existing research on rapid pyrolysis of organic solid waste and 18 sets of experimental data obtained from independent experiments. By the combination of the S-type tansig function of the hidden layer with the linear transfer purelin function of the output layer, the transfer function was created to construct the mapping between input and output variables. The results showed that when the number of hidden layer neurons was 14 and the learning rate was 0.04, the predicted yields and experimental yields were in good agreement with the R2 of neural network training and testing samples were 0.943 and 0.889, respectively. Increasing temperature and prolonging solid residence time were beneficial to the conversion of solid phase products to gas and liquid phase products. The effect of gas residence time on the three-phase yield distribution was less than that of temperature and solid residence time.

- **Keywords:** BP neural network; Multiple organic solid waste; Medical waste; Rapid pyrolysis; Yield prediction

Yijing Li, Tian Zhu, Shijia Qin, Guangzai Nong, Yongjun Yin. *Energy conservation and emission reduction of a new pulp mill by improving production processes*. Pages 662-672.

A new method of recycling cooking with pulping wastewater was developed to save energy and reduce carbon dioxide emissions in a pulp mill, which used bio-fuel of eucalyptus instead of coal and oil, and reduced the steps of black liquor combustion and lime regeneration in the traditional pulp mill to reduce carbon dioxide emission. As results, the bio-fuel consumption and CO2 emission are 2.04 × 104 MJ (1.2 tons of

eucalyptus) and 2.2 tons for per ton of pulp. It reduces 28.23% of fuel energy consumption and 14.06% of CO2 emission comparison with that by the traditional pulp mill. In addition, while using the generated lignin as part of bio-fuel, the product value-added is 765.88 RMB for per ton of pulp, being 23.72% lower than that of 1004.08 RMB by the traditional pulp mill. Therefore, this study demonstrates the advance and feasibility of using only bio-fuel for a new pulp mill with a new method of recycling cooking, and will promote the technological revolution of cleaner production in the pulp and paper industry.

- **Keywords:** Biofuel; Pulping; Recycle cooking; CO2; Product value added

Yuting Li, Ruying Li. *A hybrid model for daily air quality index prediction and its performance in the face of impact effect of COVID-19 lockdown*. Pages 673-684.

Accurate and dependable air quality forecasting is critical to environmental and human health. However, most methods usually aim to improve overall prediction accuracy but neglect the accuracy for unexpected incidents. In this study, a hybrid model was developed for air quality index (AQI) forecasting, and its performance during COVID-19 lockdown was analyzed. Specifically, the variational mode decomposition (VMD) was employed to decompose the original AQI sequence into some subsequences with the parameters optimized by the Whale optimization algorithm (WOA), and the residual sequence was further decomposed by the complete ensemble empirical mode decomposition with adaptive noise (CEEMDAN). On this basis, a deep learning method bidirectional long short-term memory coupled with added time filter layer and attention mechanism (TFA-BiLSTM) was employed to explore the latent dynamic characteristics of each subsequence. This WOA-VMD-CEEMDAN-TFA-BiLSTM hybrid model was used to forecast AQI values for four cities in China, and results verified that the accuracy of the hybrid model outperformed other proposed models, achieving R2 values of 0.96–0.97. In addition, the improvement in MAE (34.71–49.65%) and RMSE (32.82–48.07%) were observed over single decomposition-based model. Notably, during the epidemic lockdown period, the hybrid model had significant superiority over other proposed models for AQI prediction.

- **Keywords:** Air quality index; COVID-19; Two-stage decomposition; Long short-term memory; Attention mechanism

Sanjeev Kumar, Davinder Singh. *Transforming waste into sustainable solution: Physicochemical and geotechnical evaluation of cement stabilized municipal solid waste incinerator bottom ash for geoenvironmental applications*. Pages 685-695.

The present study investigates the potential of Municipal Solid Waste Incinerator Bottom Ash (MSWI-BA) collected from a waste-to-energy conversion plant in Delhi for geoenvironmental applications. The physicochemical and geotechnical properties of freshly quenched MSWI-BA were examined for cement-stabilized specimens with varying cement content ranging from 3% to 9%. The study aimed to assess the influence of pH and metal(loid)s concentrations during the standard curing period. The results demonstrated that adding cement formed C-S-H and C-A-H gel and Ca-hydrates within the matrix of 28-day cured samples. Specimens with 7% and 9% cement content exhibited the presence of quartz, calcite, belite, and other strength-enhancing compounds, leading to significant improvements in unconfined compressive strength and California bearing ratio values by up to 119.37% and 96.42%, respectively. Thermogravimetric analysis indicated moisture loss and breakdown of aluminates and silicates caused cracking at temperatures above 720 °C. The incorporation of cement resulted in the encapsulation of heavy metals, with the concentrations of Zn and Cu

remaining within permissible limits. This study confirms the applicability of cement-stabilized MSWI-BA for flexible road pavements, earth fills, and various geoenvironmental applications.

- **Keywords:** MSW-Bottom ash; Waste management; Solidification; Microstructure; Leachability

Jing Li, Guo Lin, Biao Zeng, Likang Fu, Zeying Wang, Shixing Wang, Tu Hu, Libo Zhang. Enhanced Hg(II) efficient and selective removal by post-functional Ti-MOF with 2, 5 thiophene dicarboxylic acid. Pages 696-705.

Toxic mercury ions in wastewater from industrial activities can wreak havoc on the natural environment and ecosystems. Adsorption treatment has been proved to be an effective measure to reduce mercury load in wastewater, but conventional adsorbents have lower adsorption performance. In this study, titanium-metal organic framework (Ti-MOF) was synthesized by solvothermal method, and then further modified by 2,5-thiophene dicarboxylic acid. In order to explore the morphology of the resulting material (OB-MIL-125 (Ti)) and the differences before and after modification, different characterization instruments have been employed. Meanwhile, the properties of materials at different pH were explored, and the adsorption capacity was deeply studied through thermodynamics, kinetics, and adsorption isotherms. The surface of OB-MIL-125 (Ti) had a rich pore structure, so the specific surface area is large, reaching 328.7 m2/g. At room temperature and pH= 5, the maximum removal rate of a 100 ppm solution reached 93.66%. The actual measured maximum adsorption capacity was 1435.98 mg/g. According to isotherm, kinetic and thermodynamic analysis, the process of removing Hg2+ was a multi-layer heterogeneous process, relying on chemical action for adsorption, and it was also a spontaneous exothermic process. The adsorbent presented excellent affinity for mercury and good regeneration ability. To sum up, the OB-MIL-125 (Ti) has great potential for remediation mercury-containing wastewater.

- **Keywords:** NH2-MIL-125 (Ti); Adsorption; Mercury; Wastewater

Xiaofeng Li, Guohua Chen, Paul Amyotte, Mohammad Alauddin, Faisal Khan. *Modeling and analysis of domino effect in petrochemical storage tank farms under the synergistic effect of explosion and fire*. Pages 706-715.

The synergistic effect of explosion and fire (SEEF) is one of the challenges of domino effect risk assessment for petrochemical storage tank farms. However, the domino effect probabilities at different orders and accident propagation patterns in storage tank farms under the SEEF are still unclear. An approach based on Bayesian networks is developed to model the propagation of domino effects in storage tank farms under the SEEF. The method accounts for the temporal and spatial synergistic effects of blast wave and fire thermal radiation in multiple accidents during domino accident escalation and the damage enhancement effect caused by the SEEF on the target units. Application of the method to a real tank farm highlights that the SEEF has a significant impact on the domino effect probabilities. Compared with only considering a single accident type, the SEEF leads to an increase in the domino effect probabilities of the tank farm. Installing water deluge systems and blast walls for all tanks at the same time is an effective safety measure to mitigate domino effects due to the SEEF. When safety resources are limited, the priority to equip critical tanks with water deluge systems and blast walls can also mitigate the domino effects.

- **Keywords:** Domino effect; Fire thermal radiation; Blast wave; Synergistic effect; Bayesian network; Probability analysis

Grasiele Amoriso Benedet, Alexandre Zaccaron, Jordana Mariot Inocente, Vitor de Souza Nandi, Sabrina Arcaro, Fabiano Raupp-Pereira, Dino Gorini Neto. *Mining circular economy: Potential of rice husk ash as an alternative mineral source in the production of clay ceramics using simplex design*. Pages 716-724.

To determine the feasibility of using rice husk ash (RHA) in clay ceramic production, a design of experiments (DoEs) method was employed to test 10 different formulations. The vertex formulations (from triaxial diagram) were tested to obtain their chemical (XRF), mineralogical (XRD), and thermal properties (DSC/TG). After obtaining the optimum lower and upper limits of the materials, all formulations were further evaluated in terms of particle size (>45 μm), plasticity (Atterberg), real density (helium gas pycnometry), drying shrinkage at various humidities (Bigot's curve), and technological properties exhibited after thermal processing namely, total shrinkage, water absorption index, apparent density, and diametral mechanical strength. The integration of RHA into ceramic paste showed positive impacts on the drying process and dimensional control - higher RHA content decreases shrinkage and stabilizes the drying more quickly; however, it reduced the density and plasticity of the formulations. The use of RHA > 25% left the plasticity index < 10, impairing the workability of the paste. The results of the mixture design method indicated that RHA could only be used in a limited capacity of 15% by mass; higher RHA contents would make the water absorption index exceed the threshold established as per the technical standard (25%).

- **Keywords:** Mining Circular Economy; Rice husk ash; Clay ceramic; Design of experiments

Zhenghui Wang, Jian Chen, Yueyang Yu, Depeng Kong. *Experimental study on the ignition and burning characteristics of liquid fuels on hot surfaces*. Pages 725-733.

As a typical fire accident in industrial process, the liquid fuel fire ignited by hot surfaces may pose a threat to process safety and environmental protection. Therefore, the ignition and burning characteristics on hot surfaces are investigated for different liquid fuels, including light crude oil, transformer oil, and corn oil. In the experiment, the ignition and burning characteristic are obtained and discussed, including ignition probability, ignition delay time, burning behavior and flame height. Based on the logistic regression model, the ignition probability curves with S-shaped are fitted by experimental data, and the characteristic ignition temperatures and ignition temperature regions are obtained and compared. The mathematical model is developed to explain the variation of ignition delay time with hot surface temperature. Moreover, the burning processes of the liquid fuel samples ignited by hot surfaces is analyzed and discussed, and the phenomenon of flame overflow is observed to occur in the transformer oil. Based on dimensionless analysis, the maximum flame height could be related with the hot surface temperature and ignition delay time. This work is essential to improve industrial process safety management throughout the production, storage, transportation, and utilization of liquid fuels.

- **Keywords:** Hot surface; Ignition probability; Ignition delay time; Burning behavior; Flame height

Yan Yang, Yilin Kong, Guoying Wang, Yujun Shen, Ruolan Tang, Ziming Yin, Jia Yang, Guoxue Li, Jing Yuan. *Temporal succession and spatial heterogeneity of humification, pathogens and bacterial community in facultative heap composting*. Pages 734-746.

The oxygen (O2) content of heap composting pile gradually decreased with depth, mainly because of limitations to air diffusion. Owing to uneven distribution of O2, composting

was aerobic in upper layer, facultatively anaerobic in middle layer, and anaerobic fermentation occurred in bottom layer. Therefore, this study investigated temporal succession and spatial heterogeneity of humification, pathogens and bacterial community in facultative heap composting. In this study, pig manure alone or mixed with cornstalk was composted for 90 days without ventilation or turning. Different compost layers exhibited discrepancies in maturity and bacterial community due to differences in air diffusion during heap composting. From the compost pile's upper to lower levels, the maturity of both treatments decreased from 80.60% to 0%, and the Shannon index decreased from 4.09 to 2.08. Cornstalk regulation significantly improved compost maturity and humification, brought obvious improvements to bacterial diversity and cooperative interactions and accelerated transformation from anaerobic to aerobic bacteria by enhancing porosity and oxygen diffusion. Cornstalk addition would slow the rate of pathogen reduction but could inactivate more thoroughly. The structural equation model revealed oxygen content, temperature and bacterial community mainly influenced pathogen inactivation, and key factors affecting humification were dissolved organic carbon and bacterial community.

- **Keywords:** Facultative heap composting; Bacterial dynamics; Spatial heterogeneity; Pathogens; Humification

Andreas Mack, Sonia Ruiz-Pérez, Hans Boot. *Extension of the EFFECTS dispersion model for buoyant plume rise including lift-off*. Pages 747-762.

Alternative energy carriers such as hydrogen and ammonia play an important role for the energy transition to reduce global CO2 emissions substantially. These substances will be produced and used in much larger amounts in the near future to replace hydrocarbons that are widely used nowadays. Therefore, consequences and risks of bulk storage, handling and transport of these materials must be addressed accurately. Because these substances have a low molecular weight, pressurised or liquefied gases released by accident may undergo a transition from heavy gas to rising plume behaviour during dispersion depending on the storage, release and atmospheric conditions, as well as surface effects such as heat transfer. The plume lift-off, plume rise, and the entrainment of ambient air play a significant role in the effect distances and the volume of a flammable or toxic cloud. The consequence modelling software tool EFFECTS contains different dispersion models for neutral and heavy gas dispersion, which are based on a 1-D discretisation method. Since the code for these dispersion models was developed in the past with the focus on heavy or neutral gas conditions, the simulation of buoyant plumes so far was limited. The aim of the present research was to improve the accuracy of the EFFECTS dispersion model for strongly buoyant plumes and predict the transition from the momentum dominated to the buoyant regime correctly. The paper describes the theoretical background of the extensions implemented in the dispersion model in EFFECTS. These extensions are aimed at improving the modelling approach for lighter than air plumes. The validation of the models incorporating these improvements has been performed and is based on results compared against experimental data including instantaneous and continuous releases, jets and low momentum releases from the ground for different materials including helium and hydrogen.

- **Keywords:** Buoyant plume; Plume rise; Dispersion modelling; Hydrogen; Helium; Ammonia; LNG; Consequence analysis

Gen Liu, Zhi Liu, Siwen Li, Chunyan Shi, Tongyu Xu, Mingxin Huo, Yingzi Lin. *Aluminum copper bimetallic metal organic gels/sodium alginate beads for efficient adsorption of ciprofloxacin and methylene blue: Adsorption isotherm, kinetic and mechanism studies*. Pages 763-775.

In this research, a new aluminum-copper bimetallic organic gel was prepared by solvothermal method. It is hoped that the special structure and properties of this new material can be used to remove ciprofloxacin (CIP) and methylene blue (MB) from water to deal with environmental pollution problems. Their morphology and structure were characterized by XRD, FT-IR, XPS, SEM, BET, TGA and zeta potential. It is proved that they have sufficient active sites, large specific surface area (270.5 m2/g), hierarchical porous structure, and strong thermal stability. These properties contribute to their efficient removal of pollutants. Compared with other adsorbents, MOG-4 in this study showed good pollutant removal rate, wide pH adaptability, good anti-interference ability and excellent reuse rate. The maximum adsorption capacity of MOG-4 for CIP and MB was 458.72 mg/ g and 381.68 mg/ g respectively. The adsorption process followed the second-order kinetic model and Freundlich isotherm. More importantly, we constructed MOG-4 @SA beads by immobilizing MOG-4 in sodium alginate (SA) matrix, which not only overcame the shortcomings of difficult recovery and easy agglomeration of powder MOG-4, but also enhanced its adsorption capacity. Seven cycles show that the reuse rate of MOG-4 @SA is more than 84%. The adsorption mechanism involves hydrogen bonding, electrostatic interaction, π-π interaction, hydrophilic/hydrophobic interaction and pore filling. MOG-4 @SA beads adsorbent overcomes the shortcomings of traditional powder adsorbent, which is easy to lose, easy to aggregate and difficult to recover, and broadens the range of use of powder adsorbent and sodium alginate. Therefore, MOG-4 @SA has the advantages of good adsorption performance, high reuse rate, wide range of adaptation, strong anti-interference ability, and is expected to become a promising adsorbent.

- **Keywords:** Immobilized MOGs; Electrostatic interaction; Hydrogen bonding; π-π interaction; DFT

Zegang Fu, Ye Shui Zhang, Guozhao Ji, Aimin Li. *Hydrothermal transformation behavior and degradation pathway analysis of waste surgical masks in supercritical water*. Pages 776-785.

The massive use of surgical masks around the world has exacerbated plastic pollution. Efficient treatment of these surgical masks is urgently needed. Supercritical water degradation has been considered as a promising method for treating surgical masks. In this study, analysis of the products revealed that the production rate of H2 and olefins from surgical masks with nose clips treated by supercritical water were significantly higher than that without nose clips. Therefore, it was concluded that Fe in the nose clip could catalyze the dehydrogenation of alkanes and inhibit the aromatization of cycloalkanes and alkenes compounds in the supercritical water treatment process of waste surgical masks. However, the ethylene vinyl acetate (EVA) hot melt adhesive in the surgical masks degraded at a low temperature, producing ketone compounds that negatively impacted the quality of liquid oil. This study could provide a basic understanding and effective guidance for surgical masks degradation in supercritical water.

- **Keywords:** Surgical mask; Supercritical water; Conversion behavior; Degradation

Burak Ayyildiz, M. Ziyan Sheriff, Mohammad Azizur Rahman, Adolfo Delgado, Ibrahim Hassan, Hazem Nounou, Mohamed Nounou. *Research on pinhole accidental gas release in pipelines: Statistical modeling, real gas CFD simulation, and validation.* Pages 786-796.

The successful risk mitigation of Natural Gas (NG) leakage to reduce its environmental and economic impact depends chiefly on timely detection leaks and predicting the amount of gas release. In the present study, we investigated pinhole leaks and predicted the gas release rate for various leak to pipe diameter ratios and operating pressures ranging from 2 bar to 110 bar. We first set up a laboratory-scale experiment. The generalized likelihood ratio (GLR) is used as an advanced statistical hypothesis testing technique to detect any shifts in the mean and variance of the process measurements in real-time. These results improved the understanding of several leak detection systems and contributed to a reduction in false alarms in these systems. The presence of a leak was flagged almost immediately after it occurred, indicating the speed and efficiency of statistical techniques in detecting microleaks. The present computational fluid dynamics (CFD) study provides details on the entire leak flow field that are not possible to obtain with experimental methods. CFD is a critical tool in process safety management, helping to identify, analyze, and mitigate potential risks in natural gas pipeline. The CFD study proposes new correlations to predict the nominal leak volume flow rate by investigating the influence of leak size, pipe diameter, and pipe pressure for wide ranges of pressures. The correlations were derived from three-dimensional transient detachable eddy simulation model in a commercial CFD code (ANSYS Fluent R3). The correlations enhance the conventional models by incorporating the gas compressibility effect for high-pressure conditions. The percentage of error between the results of the CFD and delivered correlation fluctuated between 4% and − 5%, demonstrating the high accuracy of the new correlation.

- **Keywords:** CFD simulation; Chronic leak detection; NG pipeline leakage; Real gas simulation; Generalized Likelihood Ratio (GLR); Numerical investigation

Ava Mokri, Arshiya Noorpoor, Fateme Ahmadi Boyaghchi. *Evaluation and multi-objective salp swarm optimization of a new solid oxide fuel cell hybrid system integrated with an alkali metal thermal electric converter/absorption power cycle*. Pages 797-816.

This research introduces a new combination of an alkali metal thermal electric converter (AMTEC) and an absorption power cycle (APC) to boost the performance of the solid oxide fuel cell (SOFC) by recovering the high-quality heat released from the SOFC for further electricity production. The performance criteria of the proposed SOFC/AMTEC/APC hybrid system are mathematically derived using thermodynamic, exergoeconomic, and exergoenvironment-based carbon footprint analysis. Extensive parametric assessment is carried out to evaluate the effect of substantial design parameters on the system's performance criteria. Furthermore, the multi-objective salp swarm algorithm (MSSA) with decision-making techniques is performed to ascertain the hybrid system's maximum power density and minimum cost and environmental impact rates densities. Findings depict the effectiveness and merit of the proposed system with 81% power density improvement compared with the related SOFC-based system. Moreover, the system yields the maximum power density of 9589.37 W/m2, and the corresponding energy and exergy efficiencies are obtained by 55.2% and 57.74%, indicating 59.26% and 53.76% improvements relative to the single SOFC. Furthermore, the minimum cost and CO2 emission rate densities are achieved by 4.26 $/h m2 and 3.32 kgCO2/h m2, respectively, with 31.73% and 42.3% enhancements relative to the base point.

- **Keywords:** Solid oxide fuel cell; Alkali metal thermal electric converter; Absorption power cycle; Exergoeconomic, environmental impact; MSSA

Zi Lin, Lin-Quan Gong, Jing-Jing Xu, Jia-Jia Jiang, Jun-Cheng Jiang. *Multi-objective optimization of chemical process plant layout considering economy and inherent safety*. Pages 817-830.

Economy and safety are important factors for the layout design of chemical process plants. However, safety factors are often translated into economic indicators as a part of the objective function for layout optimization in previous studies. This may result in safety performance of chemical process plants does not meet the actual production requirements. In this paper, a multi-objective optimization method for chemical process plant layout is proposed to obtain series of solutions that can achieve the trade-off between economy and safety. The economic objective function is characterized by the total capital cost, including land cost, pipe cost, protection device cost and expected property loss from accidents. The safety objective function involves inherent safety which is evaluated by the Comprehensive Inherent Safety Index (CISI). The proposed multi-objective optimization model solved by non-dominated sorting genetic algorithm II (NSGA-II) is applied for layout optimization of an acrylic acid production plant. The results show a strong trade-off between competing economic and safety objectives according to the Pareto curve. The optimal solution ranges from 236,099 $ to 379,622 $ for total cost, corresponding to 87.7–132 for CISI. Safety will be improved significantly in the low-safety layout scheme when the capital investment increases slightly.

- **Keywords:** Chemical process plant; Inherent safety; Layout optimization; Multi-objective optimization; Pareto curve

Kaiyu Zou, Shouxiang Lu. *Comparative study on the influence of incident heat flux on thermal runaway fire development of large-format lithium-ion batteries*. Pages 831-840.

In response to the growing demand for higher energy density in various applications, large-format batteries have gained popularity. However, the larger size of these batteries also increases their exposed area, which may lead to more severe thermal events. This study aims to understand the influence of incident heat flux on the occurrence and progression patterns of fires in large-format lithium-ion batteries. Two representative large-format lithium-ion batteries, 38 Ah LiNi0.3Co0.3Mn0.3O2 prismatic cell and 78 Ah LiNi0.8Co0.1Mn0.1O2 pouch cell, were investigated. To evaluate the thermal hazard to the environment, the heat release rates (HRR) of the lithium-ion battery fire were measured under incident heat fluxes ranging from 10 to 50 kW·m−2, using the oxygen consumption principle. The results highlight significant differences in thermal runaway and fire development between the 38 Ah and 78 Ah cells, attributable to variations in structure and materials, and scale effect. The 38 Ah cell exhibited an evident venting stage, characterized by an unignited jet on the verge of ignition, followed by a transition from momentum-driven jet fire to buoyancy-driven jet fire. In contrast, the 78 Ah cell experienced direct ignition, accompanied by strong air entrainment, overflow flame, and flame sinking phenomena as the fire progressed. Notably, unlike the 38 Ah cell, the peak HRR, THR, and burning time of the 78 Ah cell were minimally sensitivity to the incident heat flux. Furthermore, a generalized relationship model between the incident heat flux and the ignition time was established and validated based on the energy conservation equation during the ignition stage of the cell. This model enhances our understanding of the interplay between incident heat flux and ignition time, contributing to the development of strategies for fire prevention and mitigation in large-format lithium-ion batteries.

- **Keywords:** Large-format lithium-ion batteries; Thermal runaway; Heat release rate; Incident heat flux; Ignition time

Yu Huang, Jiajun Wang, He Gu, Xinpeng Zhou, Jiale Xie, Dongfeng Wang. *False data injection attack detection for nuclear reactor based on chaotic time/frequency-hopping spread spectrum*. Pages 841-851.

False data injection (FDI) attacks represent a serious threat to securing nuclear reactor operation. Efficient FDI attack detection is essential to prevent related unforeseen nuclear accidents. However, owing to their design principles, the existing detection methods are limited in their ability to detect multiple types of FDI attacks. To address this issue, we propose a detection scheme for FDI attacks on a nuclear reactor based on the chaotic time/frequency-hopping (TH/FH) spread spectrum. The proposed scheme uses frequency hopping modulation, demodulation, and filtering of the signal based on hyper-chaotic sequences to limit the attacker's access to the system's real data and eliminate the adverse effects of attacks on the system. Furthermore, theoretical analysis derives the stability constraint of the frequency hopping frequency and demonstrates the detectability and defendability of the proposed scheme. Experimental simulations demonstrated that our proposed scheme can detect two typical FDI attacks, replay attacks and covert attacks, without compromising system operation, and defend against and reproduce covert attack signals.

- **Keywords:** Nuclear reactor; Attack detection; False data injection attack; Chaotic time/frequency-hopping spread spectrum

Arash Javanmard, Wan Mohd Ashri Wan Daud, Muhamad Fazly Abdul Patah. *The good, the bad, the advantage of washing pretreatment in reducing slagging and fouling index during the torrefaction process*. Pages 852-866.

This review paper focuses on investigating the effectiveness of washing pretreatment in reducing slagging and fouling index during the combustion process of empty fruit bunches (EFB) materials. Slagging and fouling are common problems encountered in combustion systems that burn these types of materials for energy generation, leading to operational and maintenance issues. Washing pretreatment has emerged as a promising solution to mitigate these problems by removing undesirable chemical species from the biomass before combustion. This paper examines the existing literature on the effectiveness of washing pretreatment in reducing slagging and fouling index during the combustion process. The review covers various aspects, including washing methods, and combustion conditions used in previous studies. The review highlights that washing pretreatment can effectively reduce slagging and fouling index during the combustion process of EFBs. The paper also discusses the mechanisms behind the effectiveness of washing pretreatments, such as the removal of alkali and heavy metal compounds, and the reduction in ash content. Finally, the review paper provides recommendations for future research directions in this area. Overall, this study provides valuable insight into the factors, such as temperature, soak time, and water use, that can reduce slagging and fouling during the combustion process and have the potential to increase the effectiveness and dependability of energy generation systems.

- **Keywords:** Empty fruit bunches; Chemical free treatment; Slagging and Fouling problems; Ash content; Undesirable chemical species

Li Bai, Muhammad Asadollahzadeh, Bhupendra Singh Chauhan, Mostafa Abdrabboh, Mohamed Fayed, Hamdi Ayed, Abir Mouldi, Mohammad Marefati. *A new biomass-natural gas dual fuel hybrid cooling and power process integrated with waste heat recovery process: Exergoenvironmental and exergoeconomic assessments*. Pages 867-888.

The integration of gas turbine cycle (GTC)-based energy processes with a biomass gasification process employing a post-combustion approach, in addition to improving the reliability and performance of the energy cycle, can reduce the current crisis in the energy sector and balance the environmental impacts of the hybrid energy cycle. The present paper develops a multi-criteria evaluation and optimization of a novel hybrid cooling and power process (HCPP) based on GTC and post-combustion-based biomass gasification process integrated with downstream cycles. Two fuels (i.e., natural gas and biomass) are utilized simultaneously to produce energy in the proposed process. In addition, the downstream cycles are based on two organic Rankine cycles (ORCs) and a refrigeration unit to recover waste heat. The performance of the developed HCPP has been evaluated and discussed from the thermodynamic-conceptual, exergoenvironmental and exergoeconomic points of view. Additionally, a tri-objective optimization is applied to identify optimal inputs and outputs variables. The overall results indicated that the proposed HCPP can produce 13 MW of electric power and 7.6 MW of cooling load. The thermal and exergy efficiencies of the system were 70.1% and 42.85%, respectively. Moreover, the values of levelized cost of energy (LCOE) and product unit environmental impact (PUEI) were calculated as 0.0748 USD/kWh and 0.0184 Pts/kWh, respectively. However, under tri-objective optimization, the values of LCOE and PUEI can be reduced by approximately 9.4% and 16.8%. The effect of different parameters was also discussed and evaluated through a parametric analysis. Furthermore, the conceptual assessment and design of the solar field was developed for a hypothetical scenario and configuration (based on geographical conditions of a certain region).

- **Keywords:** Dual fuel; Biomass; Natural gas; Hybrid cooling and power; Waste heat recovery; Exergoenvironmental

Thangavelu Kokulnathan, Tzyy-Jiann Wang, Faheem Ahmed, Thamraa Alshahrani. *Synthesis of 3D flower-like zinc-chromium layered double hydroxides: A functional electrode material for furaltadone detection*. Pages 889-897.

Furaltadone (FLD) as an antibiotic has been widely used in animal husbandry to treat bacterial infection and promote animal growth. Its abnormal usage has threatened human health and the ecological system. The sensitive FLD detection is crucial for the protection of human health and eco-environment. In this study, unique 3D flower-like zinc-chromium layered double hydroxides (ZnCr-LDHs) are synthesized by a facile hydrothermal approach and further utilized as the electrode material for electrochemical FLD detection. The characteristics of 3D flower-like ZnCr-LDHs were systematically investigated by various microscopic and spectroscopic methods. This 3D-flower-like ZnCr-LDHs endows the electrocatalyst with rich electroactive sites, good conductivity, large surface area, and rapid ion diffusion to promote electrochemical activities. The ZnCr-LDHs modified glassy carbon electrode (GCE) shows superior electrochemical performance for the detection of FLD compared to the pristine GCE, including. wide linear ranges (0.01–60.8; 60.8–312.9 μM), low limit of detection (1.0 nM), low limit of quantitation (3.4 nM), high sensitivity (1.31 μA μM−1 cm−2), good reproducibility (4.75%), and anti-interfering ability (<±5%). The practicality of the fabricated ZnCr-LDHs/GCE was successfully confirmed by measuring FLD in the human-urine and river-water samples with acceptable recovery values (95–99%). This work opens a new perspective way for the design and preparation of novel electrode material with unique properties for boosting electrocatalysis toward electrochemical sensing applications.

- **Keywords:** Layered double hydroxides; Two-dimensional materials; Nitrofuran; Antibiotics; Growth promoter; Electrochemical sensors

Deyong Fu, Guiqiu Hu, Manoj Kumar Agrawal, Fan Peng, Badr Alotaibi, Mohammed Abuhussain, Theyab R. Alsenani. *Multi-criteria optimization of a renewable combined heat and power system using response surface methodology*. Pages 898-917.

Sun is one of the reliable sources of energy that is available in most locations in the world. Among various solar power units, the parabolic trough collector (PTC) is one of the most functional systems that can provide considerable thermal energy. However, this unit is not able to directly provide electrical energy. Thus, this study presents a non-dimension model of a renewable power system that incorporates a photovoltaic cell and a PTC unit. This hybrid system can simultaneously provide both heating load and electricity. The scheme is examined from the perspectives of exertion, energy, emission, entropy, and economics (5E). In this order, the influence of diverse operating factors on the outcomes of the unit, including saved cost, electrical and thermal exergies, CO2 emission, electrical and thermal energies, and entropy generation, are examined. On top of that, the performance of this innovative unit is optimized using both single-objective and multi-objective methods. The findings indicate that increasing fluid inlet temperature and solar radiation intensity lead to an increase in the temperature of every component of the unit. A stronger heat transfer from the receiver tube to the working fluid causes the temperature of the fluid and solid zones to decrease when the mass flow rate is increased. The analysis shows that the optimum value of solar radiation for the electrical exergy and saved cost is around 900 W/m2 and further reduction or increment in the value of this parameter has an unfavorable impact on both electrical exergy and saved cost. While, raising solar radiation improves all other output parameters of the unit, continuously. Also, it is found that the concentration ratio is the only parameter that elevation in its value leads to ascending the value of all output parameters of the presented system. Based on the findings, at the optimum operating condition, the value of saved cost, CO2 emission, and entropy generation are 70 USD/month, 803.956 kg/month, and 23.93 W/m.K, respectively.

- **Keywords:** Solar-assisted system; Combined heat and power system; Multi-objective optimization; Response surface methodology (RSM); Parabolic trough collector

Shohreh Ariaeenejad, Elaheh Motamedi, Mahyar Ramezani Tazehabad. *Effects of agro-waste resources on characteristics of Fe/nanocellulose hybrids and their applications as novel Fenton-like catalysts in dye removal from wastewater*. Pages 918-933.

Herein, a novel, effective and bio-based Fenton-like catalyst by in situ incorporation of Fe2O3 nanoparticles on the surface of nanocellulose (NCs) was synthesized from sugar beet pulp (SBP) and utilized for efficient removal of three different dyes. Firstly, different NC samples were synthesized by acid hydrolysis of two different biomass (SBP and Q-quinoa husk) at various concentrations of H2SO4. The characterization analyses of samples showed that SBP-based NCs prepared using 60% concentration of H2SO4 (1 h string at 50 °C) showed the highest crystallinity (56.7%), lowest aggregation, highest surface negative charge (−38.5 mV), and largest surface area (13.9 m2/g) compared to the Q-based NCs. Both SBP and Q-based nanocatalyst utilized for degradation of dyes (methylene blue (MB), crystal violet (CV), and congo red (CR)), and SBP-based sample (Fe/NC-S3) displayed the best results in dye removal due to its larger specific surface area (39.8 vs. 9.2 m2/g), and higher content of magnetic nanoparticles (6.7 vs. 3.7 at% of Fe) than Q-based catalyst. At optimum conditions, Fe/NC-S3 nano-catalyst (2 g/L), in the presence of H2O2 (30 mM) removed MB, CV, and CR dyes (30 mg/L), in 30 min, at

neutral pH, with 98%, 96%, and 62% removal efficiencies, respectively. Kinetic studies revealed that pseudo-first-order model was appropriate model to explain the decolorization of dyes at these conditions, and the rate constants were 0.0217, 0.018, and 0.0113 min−1 for the degradation of MB, CV, and CR, respectively. Moreover, raising the temperature from 15 ºC to 35 ºC resulted in enhancement of removal performance of nano-catalyst for all dyes. Fe/NC-S3 nano-catalyst showed proper reusability (just around 20% decrease for removal of all three dyes after ten consecutive reuse runs). Treatment of real water effluent (collected from a textile factory) containing mixture of all three dyes by Fe/NC-S3 and H2O2 approved the practical application of nano-catalyst in dye removal from complex matrixes even after nine reusing cycles. The results confirmed that SBP biomass could effectively turn to valuable NC nanocarriers for synthesis of advanced and innovative catalysts with proficient catalytic activity, stability, and recyclability.

- **Keywords:** Nanocellulose; Fenton catalyst; Agro-waste; Water remediation; Dye degradation

Mahyar Amiri, Hamed Rashidi, Maryam Dehbani. *An intensified low-energy ultrasonic plug reactor for CO2 desorption from single and novel blended absorbents.* Pages 934-944.

Ultrasound as an efficient emerging technology for CO2 desorption enhancement has attracted great attention in recent years. In the present study, a mini-plug reactor was equipped with a 28 kHz ultrasound transducer and employed for CO2 stripping from different amine-based solutions. First, 30 wt% aqueous solutions of MEA, DEA, DIPA and MDEA were investigated under the effect of desorption temperature and flow rate of the solution. 26.4% energy saving and around 70% enhancement in desorption was reached for MEA at 55℃ using ultrasound irradiation. Some novel tri-solvent blends were also studied in the optimum temperature. Among four blended amine solutions, new aqueous solution of MEA+DIPA+AMP showed the maximum desorption rate of 84.2% and minimum regeneration energy of 2.7 MJ/kgCO2 using the designed ultrasound-equipped plug reactor. It was concluded that CO2 desorption from the MEA+DIPA+AMP blend could reduce required energy consumption by around 35% compared to 30 wt% MEA using conventional method. The present study provided an efficient intensified desorber as well as a kind of tri-solvent blend as a brilliant system for CO2 capture process at lower temperature than conventional.

- **Keywords:** CO2 desorption; Regeneration; Amine solution; Ultrasound; Acoustic cavitation

Changshuai Zhang, Hongguang Dong, Sheng Shang, Kai Zhang, Yonghao Zhou, Wei Gao. *Experimental investigation of the vented propane-air explosion characteristics at elevated static activation pressures in a large L/D duct*. Pages 945-955.

The flame behavior and pressure characteristics of vented propane-air explosions at elevated static activation pressures (Pstat) were investigated in a duct with a length-to-diameter (L/D) ratio of 7. The impact of the discharge traction and the coupling effect of the internal flame front and pressure waves on the flame propagation behavior were captured. The effect of increasing Pstat on the vented flame length and width under a fixed vent was weak. The influences of Pstat on the pressure profiles and maximum reduced pressure (Pred) were investigated. The increase of Pstat mitigated the blocking effect of external explosion on Pred and further promoted the discharge pressure drop rate to be controlled within the limit of the discharge capacity of the vent. The formation mechanisms of the two main external pressure peaks were analyzed. For the larger Dv conditions, the sensitivity of high Pstat to the increase of maximum external pressure

was higher than that of low Pstat. A modified model of Pred was developed considering the effects of elevated Pstat and vent coefficient KV, which is proved to have a good performance in vented explosion ducts with a large L/D ratio.

- **Keywords:** Elevated static activation pressure; Propane-air vented explosion; Vented flame; Maximum reduced pressure; Empirical modification prediction model

Haifeng Gong, Xinxin Liang, Chen Huo, Ye Peng, Hong Yin, Bao Yu, Yan Pan, Yunqi Liu. *Effects of electric field on the filtration characteristics of solid particles in oil.* Pages 956-967.

The presence of solid particles in oil can easily lead to surface failure of machine components. In order to reduce the harmful effects of solid particles, it is necessary to remove solid particles from oil. The electrostatic method is an efficient method for removal of solid particles under an applied electric field. However, the filtration mechanism for solid particles in mixed oil–solid systems using electrostatic methods has not been fully investigated. In view of this, an oil–solid separation method based on electric field enhancement is proposed. For this method, a numerical model of oil–solid separation under different electric field strengths is established by coupling the electric and flow field governing equation, the particle-wall collision equation, and the discrete phase tracking equation. Solved by finite element method, the influence of electric field on particle motion and filtration performance of the system is studied. The results indicated that in the mixed oil–solid system, the filtration efficiency is significantly increased by more than 32.97% when an electric field is used. When E > 1 kV/mm, the flow rate of particles into and out of the filter increased with increasing electric field intensity, the deposition became more dispersed, the highest deposition concentration was 3.69 times that without an electric field, and the filtration efficiency decreases but does not exceed 10% as the flow rate increases. When the particle size is greater than 30 μm, the filtration efficiency increases by at least 14.71% for every 1 kV/mm increase in electric field strength, up to a maximum of 97.65%.

- **Keywords:** Oil–solid separation; Electric field intensity; Movement characteristics; Filtration characteristics

Li Lv, Xiangcheng Wu, Junchao Xu, Jun Zhang, Lijuan Qian. *Effects of particle's surface properties and aggregation modes on water vapor competition in heterogeneous nucleation of water vapor on the particles*. Pages 968-976.

Heterogeneous nucleation of water vapor on particles to promote particulate abatement is widely used in the fields of industrial dust removal pretreatment technology. Water vapor competition is a very important phenomenon in the process of particles nucleation, but due to the limitations of experimental methods, this phenomenon is difficult to observe and rarely received attention. Therefore, in order to reveal the influence of water vapor competition on particles nucleation, a direct visualization method based on the Environmental Scanning Electron Microscope (ESEM) is proposed in this work to obtain the water vapor competition process during particles nucleation at a microscopic scale. Firstly the effect of particle's surface structure on water vapor competition in heterogeneous nucleation of water vapor on the particles is visualized by the ESEM. The results show that the embryo appears randomly at any edge of the smooth spherical particle because water vapor competition at each point on the particle's surface is equal. While the embryo always appears on the protuberance of the convex spherical particle since water vapor competition is strongest there. Then the influence of particle's surface energy on water vapor competition is also visualized. Water vapor preferentially nucleates on the particle with smaller contact angle, which means the higher the surface

energy, the more conducive it is for water vapor competition to form embryos. Finally, the impact of particle's aggregation modes on water vapor competition is also visualized by the ESEM. The results show that when the vapor supersaturation is constant, water vapor only nucleates on the two-close and three-circled particles while particles nucleation on the single particle is never observed. This is due to the strong water vapor competition at the particle's junction, where the embryos will collide and coalesce to form an embryo larger than the critical size to activate particles nucleation. The results of this study will deepen the microscopic understanding of water vapor competition in the process of particles nucleation.

- **Keywords:** Water vapor competition; Heterogeneous nucleation; Particle's surface properties; Particle's aggregation modes; Environmental Scanning Electron Microscopy (ESEM)

Chuchai Sronsri, Wanpasuk Sittipol, Napong Panitantum. *Highly-efficient process for recovering gold from discarded mobile phones using pretreatment and mild extraction*. Pages 977-987.

Existing methods for recovering gold from electronic waste are based on mechanical and hydrometallurgy approaches. However, these methods usually use toxic chemicals and demonstrate low gold extraction efficiency (Ge) due to the negative influence of organic materials and other industrial metals also present in the waste. In this work, a more efficient and more environmentally friendly process is proposed that can achieve a high Ge from electronic waste by pre-treatment and pre-extraction before gold extraction. The powdered waste was first pre-treated by a supercritical water oxidation (SWO) process to remove organic materials and then pre-extracted using a mixture of FeCl3 and HCl to remove industrial metals. The solid powder thus produced was then re-extracted by a DMF-CuCl2-NaCl mild extraction system to complete the recovery of the gold content. Experimental results indicated that pre-treatment temperature, pre-treatment time, and the concentration of the FeCl3 and HCl solutions all significantly influenced the amount of gold extracted. The optimal parameters for achieving the highest Ge extraction (99.6%) using the DMF-CuCl2-NaCl extraction system were determined as follows: an extraction temperature of 65 °C, an extraction time of 70 min, a stirring speed of 420 rpm, a sample size of ≤ 850 μm, a solid/liquid (S/L) ratio of 1:12 g·mL−1, a CuCl2 concentration of 0.8 mol·L−1, and a NaCl concentration of 1.6 mol·L−1. After gold extraction, water was then used to precipitate the gold in the form of nanoparticles. Under optimal conditions (70%v/v water, 80 min), over 98.4% of the gold could be recovered in this way.

- **Keywords:** Electronic waste; Supercritical water oxidation; Pre-treatment; Pre-extraction; Gold extraction; Mild reaction

Qin Yang, Yingchun Yang, Yujie Zhang, Yuchun Ren, Qiru Chen, Xiaodong Fang, Shengjun Sun, Longcheng Zhang, Xuefeng Zhang, Yongsong Luo, Qian Liu, Xuping Sun. *Cobalt nanoparticles supported on porous carbon nanofiber as efficient catalyst for heterogeneous activation of peroxymonosulfate towards the degradation of organic pollutants*. Pages 988-996.

In this work, cobalt-porous carbon nanofiber (Co-PCNF) was developed as a robust catalyst for the activation of peroxymonosulfate (PMS) to eliminate organic pollutants in water. Carbamazepine (CBZ) was severed as the probe to examine the ability of Co-PCNF for activating PMS. The microporous honeycomb-like structure endowed Co-PCNF with excellent catalytic activity to activate PMS as evidenced by the rapid removal rate of CBZ (0.1269 min−1) in the existence of 0.1 g/L Co-PCNF and 0.25 g/L PMS. The degradation rate of CBZ can be maintained at 89 % after five runs and the leaching concentration of

Co2+ can be neglected, suggesting the extraordinary stability of Co-PCNF reuse. Meanwhile, this system was used to degrade other organic contaminates and achieved satisfactory results, confirming the good universality of Co-PCNF/PMS system. Furthermore, the effects of catalyst and PMS dosage, pH, and co-existing ions on CBZ removal were discussed. Finally, radical identification results prove that SO4·−,·OH, 1O2, and O2·− are generated during the process of PMS activation, and a possible activation mechanism is proposed based on the aforementioned findings. This study can not only provide a method for organic pollutants elimination, but also offer a reference for designing robust heterogeneous PMS catalysts.

- **Keywords:** Cobalt nanoparticles; Porous carbon nanofiber; Heterogeneous activation; Peroxymonosulfate; Carbamazepine

Kaihao Hou, Xi Luo, Muxiang Liang, Xiaoming Liu, Qi Xu, Jing Chen, Xiejuan Lu, Xiaohui Wu, Feixiang Zan. *Heat-enhanced sulfite pretreatment improves the release of soluble substances and the stimulation of methanogenic pathways for anaerobic digestion of waste activated sludge.* Pages 997-1006.

Waste activated sludge pretreatment is effective in improving sludge hydrolysis rate and methane production. Our previous study revealed that sulfite could be a viable method for sludge pretreatment. To further improve methane production, this study employed an integrated strategy by combining sulfite and heat pretreatment. WAS from a local full-scale plant was pretreated with heat-enhanced sulfite pretreatment (HESP) at 25, 35, 55 °C. Compared with the control (no sulfite, 25 °C), soluble substances (e.g., chemical oxygen demand, protein, polysaccharides, nitrogen and phosphorus) could be significantly enhanced by the absence of sulfite and the increasing temperature. A variation of − 8.32–19.90% in cumulative methane production was observed. Moreover, methane production could be significantly enhanced by 14.15% at sulfite of 300 mg S/L and temperature of 35 °C, while kinetic analysis showed that the highest methane production potential (1.43 times of the control) was obtained at this level. Besides, the microbial structure and pathways reveal that HESP promotes the enrichment of methanogenic bacteria and facilitates methanogenic metabolism. The findings of this study suggest that the HESP could be promising in enhancing methane production, particularly considering the reuse of sulfite-laden industrial wastes and the heat as the by-products of the anaerobic digestion plant with biogas power generation, but certain experimental conditions should be verified case by case.

- **Keywords:** Sulfite; Anaerobic digestion; Methane; Waste activated sludge; Heat

Pan Yang, Lang Liu, Yonglu Suo, Mengbo Zhu, Geng Xie, Shunchun Deng. *Mechanical properties, pore characteristics and microstructure of modified magnesium slag cemented coal-based solid waste backfill materials: Affected by fly ash addition and curing temperature*. Pages 1007-1020.

The high-temperature, deep-well environment can affect the mechanical properties and long-term stability of modified magnesium slag cemented coal-based solid waste backfill material (MMS-CBM). The purpose of this study was to investigate the effects of fly ash addition (0 %, 10 %, 20 %, 30 % and 40 %) and curing temperature (20 °C, 30 °C and 40 °C) on the mechanical properties, pore characteristics and microstructure of MMS-CBM. Based on this, relevant laboratory tests (uniaxial compressive strength test, pore structure test and microstructure test) were conducted to characterize the influence mechanism of fly ash addition and curing temperature on the performance of MMS-CBM. The results show that the physical properties (uniaxial compressive strength, pore characteristics and microstructure) of MMS-CBM are significantly affected by fly ash

addition and curing temperature. With the increase of fly ash addition, the number of active particles and hydration products involved in the hydration reaction gradually increased, and the physical properties of MMS-CBM were gradually optimized. With the increase of curing temperature, the hydration reaction rate and hydration reaction degree of MMS-CBM gradually deepened, which accelerated the volcanic ash reaction of fly ash particles, which had a promoting effect on the early intensity of MMS-CBM. However, the subsequent strength of MMS-CBM will be affected by thermal damage, resulting in deterioration of physical properties and seriously affecting the long-term stability of MMS-CBM. In addition, the porosity and fractal dimension of MMS-CBM are linearly related to the uniaxial compressive strength, indicating that the pore characteristics can reflect the mechanical properties of MMS-CBM. This study provides a theoretical reference value for the application of MMS-CBM in high-temperature deep wells.

- **Keywords:** Full solid waste backfill material; Fly ash addition; Curing temperature; Uniaxial compressive strength; Pore characteristics; Microstructure

Amirah Azzouz, Maan Hayyan. *Are deep eutectic solvents biodegradable?* Pages 1021-1025.

Recently, deep eutectic solvents (DESs) have gained immense attention and consideration as a "greener" alternative to conventional volatile organic compounds and even ionic liquids. They have been marketed as cost-effective, environmentally benign, non-toxic, and biodegradable. However, most of the studies carried out on DESs have been dedicated to their physicochemical properties and their numerous applications; the evaluation of their biodegradability and environmental impact is still limited. It has been shown that depending on the choice of individual constituents used to prepare a DES, some of them cannot be simply deemed biodegradable. With the lack of attention toward the biodegradability of DESs and their fate, a short communication is needed that sheds light on their current status and elaborates on the biosafety issue. Thus, this work highlights key research efforts to date concerning DES biodegradability with the purpose of providing insight into directions for improving the sustainability of DESs and lowering their environmental impact, an essential task that will open doors for their large-scale application in a variety of industries.

- **Keywords:** Biodegradability; Green chemistry; Ionic liquid; Biocompatibility; Toxicity; Biosafety

Feng Chen, Wei Zhang, Yi Liu, Jie Cai, JinLing Zhang, XunMing Wang, Qiaolin Su. *Simulation and 4E analysis of a novel trigeneration process using a gas turbine cycle combined with a geothermal-driven multi-waste heat recovery method*. Pages 1026-1047.

A novel hybrid system using geothermal energy and fuel gas in a co-feed structure is proposed. The main objectives include improving the sustainability of a gas turbine cycle associated with a geothermal power plant and reducing carbon emissions. To this end, a novel multi-waste heat recovery process was developed in which the heated airflow in the gas turbine cycle was directed to the geothermal flash cycle to increase the viability of the flash process in this unit. A parallel heat recovery structure then used part of the waste heat from the gas turbine cycle to start a supercritical carbon dioxide cycle and also improve the performance of the geothermal flash cycle. Hence, two organic Rankine cycles were used in the geothermal flash cycle. The other part of the waste heat from the gas turbine cycle was consumed in a cascade framework in a steam Rankine cycle and a desalination plant in combination with a domestic water heater. The defined structure was simulated and a comprehensive study was done from the viewpoints of energy, exergy, environment, and thermoeconomics. This structure reduced the total irreversibility as well as the carbon dioxide emissions compared to the existing literature data.

- **Keywords:** Gas turbine cycle; Geothermal energy; Carbon dioxide emissions, Aspen HYSYS; Waste heat recovery; Trigeneration system

Alain Islas, Andrés Rodríguez Fernández, Covadonga Betegón, Emilio Martínez-Pañeda, Adrián Pandal. *Biomass dust explosions: CFD simulations and venting experiments in a 1 m3 silo*. Pages 1048-1062.

This study presents CFD simulations of biomass dust explosions in a newly developed experimental 1 m3 silo apparatus with variable venting, designed and fabricated to operate similarly to the explosivity test standards. The aim of the study is to validate a CFD model under development and investigate its capability to capture the transient effects of a vented explosion. The model is based on OpenFOAM and solves the multiphase (gas-particle) flow using an Eulerian-Lagrangian approach in a two-way regime. It considers the detailed thermochemical conversion of biomass, including moisture evaporation, devolatilization, and char oxidation, along with the homogeneous combustion of gases, turbulence, and radiative heat transfer. The explosion is analyzed in all stages, i.e., dust cloud dispersion, ignition, closed explosion, and vented explosion. The results indicate excellent agreement between the CFD model and experimental tests throughout the sequence. Our findings highlight the critical role of particle size in dust cloud distribution and pre-ignition turbulence, which significantly influences flame dynamics and the explosion itself. This model shows great promise and encourages its application for future investigations of biomass dust explosions in larger-scale geometries, especially in venting situations that fall out of the scope of the NFPA 68 or EN 14491 standards, and to help design effective safety measures to prevent such incidents.

- **Keywords:** Vented dust explosions; Biomass; CFD; OpenFOAM

Junhui Gong, Bo Liu, Haochen Lian, Jingyi Liu, Hui Fu, Yuxuan Miao, Jialong Liu. *Numerical investigation of suppressing thermal runaway propagation in a lithium-ion battery pack using thermal insulators*. Pages 1063-1075.

Thermal runaway propagation (TRP) in a lithium-ion battery pack is crucial to its safety concerning the potential hazards of fire or explosion. In current study, a TRP suppression method for a 4 × 4 battery pack using three insulation materials, silicate, ceramic and glass fiber boards, is numerically investigated. Reliability of the model is first verified by experimental temperature of a single battery during TR. Then, three sets of TRP scenarios initiated by external heating are studied to reveal the effects of insulation type, thickness (0.5–4 mm) and layout. The results show that thermal conductivity of insulation impacts its performance more greatly than thickness, and glass fiber outperforms silicate and ceramic fibers in preventing TRP. Bidirectional layout (BL) of insulation boards performs better than unidirectional layout (UL). For UL, row-to-row TRP exists and the TRP process is accelerated compared with non-insulation case if insulation boards fail, implying UL can prevent TRP only if the row-to-row TRP is inhibited. While for BL, TRP is only observed for 0.5 mm silicate fiber boards, and the critical heating power (6.5 kWm−2) triggering TRP in battery pack is much lower. The outcomes may provide useful theoretical bases and suggestions for safety design and risk assessment of battery pack.

- **Keywords:** Lithium-ion battery pack; Thermal runaway propagation suppression; Thermal insulation boards; Numerical simulation; Temperature evolution

Cong Ma, Xinbin Guo, Tong Li, Xi Jiang, Liang Wang, Bin Zhao, Zhaohui Zhang. *Anion exchange resin/quartz sand bi-layer composite dynamic membranes in ultrafiltration for algae-laden water treatment*. Pages 1076-1088.

Ultrafiltration treatment of algae-laden water is the biggest challenge of membrane fouling. In this study, a bi-layer composite dynamic membrane was constructed by depositing anion exchange resin (AER) and quartz sand on the surface of UF membrane to enhance the separation performance and reduce membrane fouling. AER deposition layers improve contaminants removal and reduce membrane fouling based on retention and ion exchange effect, however, the large porosity results in less than optimal efficiency gains. Deposition of quartz sand on the AER deposit layer significantly enhanced pollutants removal rate and reduced the fouling resistance of the membrane. Compared to AER deposition alone, the bi-layer significantly improved the removal of DOC (20%), UV254 (22%), protein (18%), polysaccharide (13%), MC-LR (11%), GSM (18%) and 2-MIB (3%) and slowed down the development of fouling resistance when the amount of quartz sand deposited reached 68.6 g/m2. As the quartz sand deposition increased to 91.4 g/m2, the presence of a critical value was found, and although the pollutants retention rate increased further, reversible fouling appeared to increase. SEM image analysis of the dense sediment layer traps too much contaminants, resulting in a gel-like layer of contamination that increases membrane fouling.

- **Keywords:** Algae-laden water; Anion exchange resin; Quartz sand; Bi-layer composite dynamic membrane; UF

Aida M. Díez, Virgínia Cruz Fernandes, Manuela M. Moreira, M. Pazos, M.A. Sanromán, T. Albergaria, C. Delerue-Matos. *Nano-zero-valent particles synthesized with agroindustry wastes for pesticide degradation under real conditions*. Pages 1089-1100.

Nano-zero-valent particles (NZVP) had exhibited high degradation activity. NZVP synthesized from agroindustry residues align with circular economy principles. They generate hydroxyl radicals (4.6 μM) that effectively degraded chlorpyrifos-methyl pesticide under real conditions. Bimetallic NZVP, specifically NZVP-Fe:Mn and NZVP-Fe:Ag, show superior pesticide degradation. The metal ratio within NZVP influences their activity (optimal at 0.12:0.12 mM and 0.12:0.19 mM for respectively, NZVP-Fe:Mn and NZVP-Fe:Ag). NZVP characterization includes TEM, SEM-EDS, PZC, FTIR, XRD, and electrochemical analysis, confirming their acid nature, favorable electrochemical behavior, and uniform metal distribution. The impact of different natural extracts on NZVP synthesis and pesticide degradation was explained through extensive extract characterization, revealing the presence of altering pro-oxidants and scavenger species. Blueberry pruning extract yields the highest pesticide degradation (85% in 5 min) due to its stronger antioxidant activity and lower scavenger compound content. NZVP demonstrates efficacy across various pH ranges. Real wastewater samples were treated under optimal conditions, resulting in a pesticide degradation efficiency of approximately 60% within 5 min. The most effective approach for enhancing the treatment process involved the sequential addition of reagents, as opposed to the conventional method of increasing reagent concentration.

- **Keywords:** Natural reductants; Photo-degradation; Pesticide removal; Low concentration; Nanoparticles

Parthasarathy Murugesan, P.V. Elumalai, Dhinesh Balasubramanian, S. Padmanabhan, N. Murugunachippan, Asif Afzal, Prabhakar Sharma, K. Kiran, JS Femilda Josephin, Edwin Geo Varuvel, Thanh Tuan Le, Thanh Hai Truong. *Exploration of low heat rejection engine characteristics powered with carbon nanotubes-added waste plastic pyrolysis oil*. Pages 1101-1119.

Compression ignition (CI)-powered alternative energy sources are currently the main focus due to the constantly rising worldwide demand for energy and the growing industrialization of the automotive sector. Due to their difficulty of disposal, non-degradable plastics contribute significantly to solid waste and pollution. The waste plastics were simply dropped into the sea, wasting no energy in the process. Attempts have been made to convert plastic waste into usable energy through recycling. Waste plastic oil (WPO) is produced by pyrolyzing waste plastic to produce a fuel that is comparable to diesel. Initially, a standard CI engine was utilized for testing with diesel and WPO20 (20% WPO+80% diesel). When compared to conventional fuel, the brake thermal efficiency (BTE) of WPO20 dropped by 3.2%, although smoke, carbon monoxide (CO), and hydrocarbon (HC) emissions were reasonably reduced. As a result, nitrogen oxide (NOx) emissions decreased while HC and CO emissions marginally increased in subsequent studies utilizing WPO20 with the addition of 5% water. When combined with WPO20 emulsion, nanoadditives have the potential to significantly cut HC and CO emissions without impacting performance. The possibility of incorporating nanoparticles into fuel to improve performance and lower NOx emissions should also be explored. In order to reduce heat loss through the coolant, prevent heat transfer into the cylinder liner, and increase combustion efficiency, the thermal barrier coating (TBC) material is also coated inside the combustion chamber surface. In this work, low heat rejection (LHR) engines powered by emulsion WPO20 containing varying percentages of carbon nanotubes (CNT) are explored. The LHR engine was operated with a combination of 10 ppm, 20 ppm, and 30 ppm CNT mixed with WPO20. It was shown that while using 20 ppm of CNT with WPO20, smoke, hydrocarbons, and carbon monoxide emissions were reduced by 11.9%, 21.8%, and 22.7%, respectively, when compared to diesel operating in normal mode. The LHR engine achieved the greatest BTE of 31.7% as a result of the improved emulsification and vaporization induced by CNT-doped WPO20. According to the study's findings, WPO20 with 20 ppm CNT is the most promising low-polluting fuel for CI engines.

- **Keywords:** Waste plastic oil; Nanoadditive; Pyrolysis process; Low heat rejection engine; NOx reduction

Matthijs van Wingerden, Trygve Skjold, Dirk Roosendans, Antoine Dutertre, Andrzej Pekalski. *Chemical inhibition of hydrogen-air explosions: Literature review, simulations and experiments*. Pages 1120-1129.

This paper summarises the first results from the joint industry project (JIP) 'Risk-reduction for hydrogen installations by partial suppression of explosions' (HyRISE). The main objective of the project is to develop fundamental knowledge that can support the development of practical solutions for mitigating hydrogen explosions in congested and confined environments by means of active systems for chemical inhibition. The aim is not to extinguish the incipient flame, but rather to lower the reactivity of the fuel-air mixture prior to ignition, and thereby reduce the consequences of an accidental explosion to a tolerable level. The paper consists of three parts: a review of previous work on chemical inhibition of premixed hydrogen-air flames, simulations with the chemical kinetics software Cantera, and experiments conducted in a 20-litre explosion vessel. The results demonstrate that chemical inhibition can be effective for hydrogen-air mixtures. However, it remains to develop efficient inhibitors and practical systems that can be

implemented in industrial facilities, with satisfactory performance over a wide range of hydrogen concentrations.

- **Keywords:** Hydrogen safety; Inhibitors; Hydrogen-air combustion