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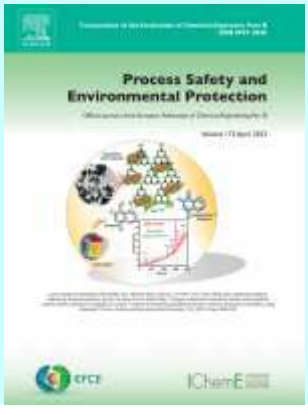

Antonio Trinca, Andrea Liberale Rispoli, Vittoria Sapone, Roberto Bubbico, Giorgio Vilardi. *Combined clean hydrogen production and bio-active compounds recovery from spent coffee grounds. A multi-perspective analysis*. Pages 1-12.

This study deals with the process simulation of an integrated system for energy production and valuable compounds recovery from spent coffee ground biomass and plasmix (non-recyclable plastic waste). The devised process consists of three maine units: a sub-critical water extraction column for the recovery of bio-compounds, an oxy-combustor of residual biomass and plasmix streams coupled with a production power energy unit, and a solid oxide electrolyzer (SOEC) for the production of pure H2 and O2. The process was exhaustively analyzed from an energy, exergy, environmental and economic point of view. The results of the analysis provided energy and exergy efficiencies higher than 60%, and the environmental analysis (CO2-cycle analysis) demonstrated a significant advantage of the process with respect to other hydrogen production methods. Finally, the feasibility of a plant with no net Greenhouse Gas emissions was shown to markedly depend on the costs associated to renewable energy sources.

- **Keywords:** Hydrogen; Waste recovery; Renewable-energy sources; Waste-to-power; Electrolysis; CO2

Duoduo Liu, Lei Zhang, Tong Zhu, Youzhao Wang, Baorui Liang, Fei Kang. *Biomass-sulfur-based mixotrophic denitrification (BSMD) process for synthetic and real wastewater treatment: Engineering application, applicable scope, and operational strategy*. Pages 13-21.

Elemental-sulfur-driven autotrophic denitrification (ESDAD) process is widely used in sewage treatment, while its low denitrification capacity has become the bottleneck of this technology. The biomass-sulfur-based mixotrophic denitrification (BSMD) process is a promising denitrification pathway to improve nitrate removal of sewage. Based on previous research, a comparative analysis of the ESDAD and BSMD processes was adopted in this study. Then, three lab-scale reactors were constructed with various BSMD

filters to investigate the characteristics of the BSMD process, and the optimal BSMD filter (F3) with the nitrate removal rate (NRR) of 556 ± 13.6 mg NO3−-N·L−1·d−1 was 3:1:1 by weight ratio of sulfur powder to rice straw powder to shell powder. Additionally, a pilot-scale reactor (volume: 1000 L) filled with filter F3 was designed and operated to treat the effluent of a municipal secondary tank. The feasibility of the BSMD process in engineering application was demonstrated, accompanied by a desirable treatment capacity (hydraulic retention time (HRT) ≤ 1 h) under varying conditions. Moreover, autotrophs and heterotrophs co-existed along the pilot-scale reactor, and the autotrophs remained dominant at seasonal temperatures. In general, the prospect of the BSMD is attractive, and the outcomes of this study could provide guidance for the operation of the BSMD process.

- **Keywords:** Biomass-sulfur-based mixotrophic denitrification; Denitrification pathway; Elemental-sulfur-driven autotrophic denitrification; Engineering application; Rice straw

Qi Guo, Ethan S. Hecht, Myra L. Blaylock, Jessica G. Shum, Cyrus Jordan. *Physics model validation of propane and methane for Hydrogen Plus Other Alternative Fuels Risk Assessment Models (HyRAM+)*. Pages 22-38.

HyRAM+ is a toolkit that includes fast-running models for the unconstrained (i.e., no wall interactions) dispersion and flames for non-premixed fuels. The models were developed for use with hydrogen, but the toolkit was expanded to include propane and methane in a recent release. In this work we validate the dispersion and flame models for these additional fuels, based on reported literature data. The validation efforts spanned a range of release conditions, from subsonic to underexpanded jets and flames for a range of mass flow rates. In general, the dispersion model works well for both propane and methane although the width of the jet/plume is predicted to be wider than observed in some cases. The flame model tends to over-predict the induced buoyancy for low-momentum flames, while the radiative heat flux agrees with the experimental data reasonably well, for both fuels. The models could be improved but give acceptable predictions for propane and methane behavior for the purposes of risk assessment.

- **Keywords:** Dispersion; Flames; Modeling; Hazards; Propane; Methane; Natural gas; Alternative fuels

Chengzhu Wang, Zhijie Wang, Keke Huang, Yonggang Li, Chunhua Yang. *Digital twin for zinc roaster furnace based on knowledge-guided variable-mass thermodynamics: Modeling and application*. Pages 39-50.

Roaster furnace is a large-scale equipment in zinc smelting process, which plays an significant role in safety production and enviromental protection. An accurate digital twin of roaster furnace can help to explore the influence of control parameters and serve as a test platform to verify the effectiveness of control strategies. However, the traditional thermodynamics cannot be used for dynamic modeling, and inability to measure key data greatly affects the accuracy of kinetic modeling. Therefore, this paper establishes a novel digital twin of zinc roaster furnace based on knowledge-guided variable-mass thermodynamics. First, based on the integration of mechanism analysis for mass balance and energy balance, a dynamic modeling method is proposed. Then, particle swarm optimization (PSO) algorithm is introduced to optimize the parameters of conversion rates guided by knowledge. Finally, by connecting the dynamic model with distributed control system (DCS) through OPC communication protocol, a digital twin of roaster furnace is constructed. Extensive experiments show that the simulation results of the digital twin roughly agree with the actual industrial data under steady and dynamic working conditions, and the application of the digital twin on the performance analysis of

control parameters and testing of control strategies can provide guidance for the optimal control of roaster furnace.

- **Keywords:** Digital twin; Zinc roaster furnace; Dynamic modeling; Variable-mass thermodynamics; Knowledge-guided

Xinxin Li, Yibao Chen, Dayue Hu, Shuang Wang, Xiangmin Li, Huanchun Chen, Ping Qian. *Novel bacteriophage-mediated β-lactamase-encoding genes and their risk assessment in environmental communities*. Pages 51-60.

Bacteria can obtain antibiotic resistance genes (ARGs) through multiple transmission routes, including horizontal gene transfer mediated by phages. Sequence-based metagenomics can detect novel phage-derived ARGs and avoid spending a great deal of time on phage isolation. Here, a metagenomic method was applied to explore the presence of ARGs in phages in freshwater samples. Two novel β-lactamase-encoding genes, blaORF88 and blaORF47, were identified and characterized in phage genomes for the first time in this study. Phylogenetic analyses indicated that blaORF88 is a member of the class C β-lactamase family, while blaORF47 formed an independent branch away from the class C β-lactamases. The average absolute abundance of blaORF88 in phage DNA and bacterial DNA was as high as 5.14 log GC/100 ml and 5.73 log GC/ml, respectively. The blaORF47 gene detected in bacterial DNA was found at the highest concentration, particularly in urban sewage samples, with 5.32 log GC/ml. Our findings raise concerns that phages might carry unknown or novel ARGs, which may spread into bacteria, leading to the emergence of antibiotic-resistant bacteria in the environment, and we urgently need effective strategies to avoid the health risks caused by ARGs.

- **Keywords:** Antibiotic resistance genes; β-lactamases; Bacteriophage; Environmental communities; Health risk

Zhidong Tang, Yuexin Han, Yue Cao, Yongsheng Sun, Peng Gao. *Clean recycling of low-grade refractory limonitic waste using suspension magnetization roasting coupled with magnetic separation: A semi-industrial approach towards a waste utilization plan*. Pages 61-74.

Efficient utilization and clean recycling of low-grade refractory iron ore are essential to deal with the fast depletion of high-grade iron ore. A semi-industrial test of suspension magnetization roasting (SMR) for a low-grade refractory limonite waste with a grade of 32.46% by using reducing gases of CO and H2 mixture was conducted. The optimal experiments conditions were determined at a temperature of 550 °C, a reducing gas flow of 3.3 m3/h, a reductant concentration of 30% and a total gas volume of 14.0 m3/h. The iron grade of 59.27% and a recovery of 96.30% were obtained in the semi-industrial continuous and stable operation experiment. The iron transformation was mainly in the order of mFe2O3·nH2O to Fe3O4, which was detected by X-ray diffraction and the relative resonance area of magnetite and γ-Fe2O3 phase was 93.90% according to the result of 57Fe Mössbauer spectral analysis. The peak of Fe3+ shifted to 710.11 eV and the area increased constantly, showing that the surface of Fe3O4 occurred in the X-ray photoelectron spectroscopy. The magnetic magnetization transformed from 0.1 to 27.71 A·m2·kg−1 using the vibrating sample magnetometer (VSM). Cracks and a large number of holes in the roasted ores could be discovered by scanning electron microscopy (SEM) and the enrichment of iron elements could be reserved by mapping scan using energy dispersive spectrometry (EDS). The environmental protection methods of the SMR was investigated by discussing the carbon emissions challenges and exhaust pollution emission problems. This study demonstrates that the SMR is a green and effective technology for low-grade limonite waste utilization.

- **Keywords:** Low-grade refractory limonite; Waste utilization; Magnetization roasting; Semi-industrial test; Magnetic separation

Nimesha Rathnayake, Savankumar Patel, Ibrahim Gbolahan Hakeem, Jorge Pazferreiro, Abhishek Sharma, Rajender Gupta, Catherine Rees, David Bergmann, Judy Blackbeard, Aravind Surapaneni, Kalpit Shah. *Co-pyrolysis of biosolids with lignocellulosic biomass: Effect of feedstock on product yield and composition*. Pages 75-87.

Co-pyrolysis technology is an effective method to reduce heavy metal concentration in biochar produced from biosolids. In the current study, the effect of co-pyrolysis feedstock on product yield and properties was studied by mixing Biosolids (BS) with Wheat Straw (WS) and Canola Straw (CS) in a 3:1 mass ratio and carrying out thermal decomposition at 700 °C in a fluid bed reactor. This study found that the feedstock ash content and the volatile matter had a significant effect on biochar, oil, and gas yields from co-pyrolysis. The results also indicated that the addition of WS and CS feedstock notably reduced As, Cd, Cr, Cu, Ni, Pb, Se, and Zn concentrations in the biochar, due to the net effect of dilution and synergistic effects. BS-WS and BS-CS co-pyrolysis reduced Cu concentration in biochar by 61.6% and 63.3%, respectively, and Zn concentration by 66.4% and 64.4%, respectively. Lignocellulosic biomass addition also reduced biochar yield and improved C, H, and N content, along with the calorific value and the thermal stability of biochar. C content was increased by 36.9% in BS: WS biochar and 43.3% in BS: CS biochar compared to solely biosolids' biochar. The calorific value of biochar was increased by 43.5% and 52.9% in BS-WS biochar and BS-CS biochar compared to biosolids' biochar. During co-pyrolysis, CS addition produced oil with the lowest mole percentage of nitrogenated compounds. However, the addition of WS and CS increased co-pyrolysis oil acidity. Biosolids co-pyrolysis with WS and CS also increased the gas yield and the heating value compared to biosolids pyrolysis. Furthermore, the synergistic effect between biosolids and co-feedstocks resulted in increased gas yields and decreased oil and biochar yields.

- **Keywords:** Biosolids; Lignocellulosic biomass; Co-pyrolysis; Biochar

Ceyhun Baydar, Hüseyin Yağlı, Yıldız Koç, Ali Koç, Sultan Büşra Artaş. *Performance and environmental improvements of a geothermal power plant by using structural and operational modification techniques*. Pages 88-105.

Performance data from a geothermal power plant that uses a dry-type working fluid (n-Pentane) was evaluated. The experimental working conditions of the geothermal power plant were recorded. By using these recorded data the structural and parametrical optimisation of the plant was applied. As a structural modification, the probable performance of the plant was scrutinised by considering the integration of a superheater into the plant. For both present and structurally optimised cases, parametric optimisations were made as an operational modification. During the analyses, the high and low pressure Organic Rankine Cycles (ORCs) of the energy converter plant were optimised for varying turbine inlet temperatures and pressures. After comprehensive analyses, it was concluded that superheating the working fluid by structural modification (superheater integration) had a negative effect on the system performance. On the other hand, together with parametric analyses, a considerable improvement in system performance was obtained. For all cases and parametric values, the system was also evaluated in terms of environmental effect.

- **Keywords:** Geothermal power plant; Ormat energy converter (OEC); Binary cycle; Low temperature heat source; Structural modification; Operational modification

Federica Ricci, Valeria Casson Moreno, Valerio Cozzani. *Natech accidents triggered by cold waves*. Pages 106-119.

Natural events are a widely recognized hazard for industrial sites where relevant quantities of hazardous substances are handled, due to the possible generation of cascading events resulting in severe technological accidents (Natech scenarios). To date, research efforts were mainly dedicated to the study of Natech scenarios triggered by earthquakes, floods, and hurricanes. However, a number of recent events evidenced the potential hazard of Natech scenarios triggered by cold waves and winter storms. The present study aims at providing a comprehensive analysis of past accidents involving hazardous substances triggered by cold waves affecting the industrial infrastructure. A dataset of over 740 Natech events was collected from specialized sources. A detailed analysis of the primary events and damage modes of the equipment items involved was carried out, highlighting that most of the accidents were linked to the phase transition from the liquid to the solid state of the process fluid or of atmospheric water. The analysis of the events allowed the identification of several aspects of the cause-consequence chains, such as the technological scenarios and the equipment items more frequently involved. A specific focus was also on the vulnerability and failure modes of safety barriers. The lessons learned derived from the analysis of the accidents provide key elements to prevent similar accidents from happening in the future. These were used to suggest specific safety barriers integrating winterization and freeze protection programs.

- **Keywords:** Natech; Major accidents; Cold wave; Database; Lessons learned; Safety barriers; Winterization

Wenshi Liu, Yu Liu, Ying Xiong, Xiao Xiao, Chunyan Liu, Bo Yuan, Xunchi Pu. *Performances and mechanisms of ferrate(VI) oxidation process for shale gas flowback water treatment*. Pages 120-130.

The aim of this study was to determine effective and green methods for the removal of organic matter from shale gas flowback water (SGFW). The effects of ferrate (Fe(VI)), initial pH, and reaction time on the removal efficiency of Fe(VI) were investigated. A chemical oxygen demand removal efficiency of 57 % was achieved under the optimal conditions of Fe(VI)= 1500 mg/L, pH= 8.0, T = 25 °C, 60 min. Combined with the results of the chemical probe method, competitive kinetic experiments, electron spin resonance spectra, and radical quenching studies, hydroxyl radicals (·OH) were demonstrated as the dominant reactive species responsible for oxidation. Furthermore, the fluorescence intensity of soluble microbial by-product-like matter and acid-like components were found to be reduced by 64 % and 43 %, respectively, using fluorescence excitation-emission matrix spectroscopy tests. The results of gas chromatography-mass spectrometry and liquid chromatography-mass spectrometry indicated that electron-rich organic compounds were easily removed by Fe(VI) oxidation. Bacterial culture and coagulation experiments showed that Fe(VI) had both disinfection and coagulation effects in the SGFW. Furthermore, considering H_2O_2 as a precursor for ·OH generation, the combined H_2O_2-Fe(VI) process was investigated in this study, and the results showed that the process has a synergistic effect and can increase the Chemical Oxygen Demand (COD) removal up to 68 % (Fe=1500 mg/L, pH=8.0, H_2O_2 =0.05 mol/L, T = 25 °C). Finally, an ultrafiltration membrane fouling experiment proved that the oxidation processes can increase the membrane-specific flux and alleviate fouling resistance. This study provides a reference for the design and operation of organic removal process in the SGFW treatment.

- **Keywords:** Shale gas; Flowback water; Ferrate; Oxidation; Hydrogen peroxide

Saba Nasiri, Ahmad Hajinezhad, Mohammad Hossein Kianmehr. *Increasing the efficiency of municipal solid waste energy by investigating the effect of die temperature and retention time on the produced pellets: A case study of Kahrizak, Iran*. Pages 131-142.

In order to optimize waste production and address the global energy crisis, the conversion of waste into energy has become a necessary practice. This study aimed to investigate fuel pellet production from unused waste at the Kahrizak Waste Center in Tehran, Iran. Pellets were produced in the laboratory as single pellets, and the impacts of two variables including die temperature (90 °C and 110 °C) and retention time (5 s and 20 s) on density, toughness, water resistance time, density change, proximate analysis, calorific value, and energy consumption producing single pellets were evaluated. The appearance of pellets indicated that higher temperatures have more effect on pellet coherence than retention time. The solid waste was shredded to fluff, and the fluff waste bulk density and heating value were measured at 30.3 kg/m³ and 12 MJ/kg, respectively. By converting fluff to pellets, the density and heating value were increased. The highest density and heating value was for pellets made at 110 °C and 5 s, and they were 883.70 kg/m³ and 29.01 MJ/kg, respectively. Additionally, retention time was the main factor influencing the total amount of energy consumption. Pellets produced at high temperatures and retention times had higher toughness up to 1696.29 J/m³ . A longer retention time in the die reduced the rate of density changes. In conclusion, considering the characteristics of the pellets and the amount of energy consumed, fuel pellets produced at 110 °C and 5 s were the best option for converting unused waste into a high-value pellet in the Kahrizak waste center.

- **Keywords:** Agglomeration; Municipal solid waste; Pellet; Refuse-Derived Fuel (RDF)

Binbin Huang, Min Gan, Zhiyun Ji, Xiaohui Fan, Guojing Wang, Zengqing Sun, Qianqian Zhao, Yufeng Wu, Siping Lu. *Co-treating MSWI fly ash in iron ore sintering process: Influence of water-washing and roll forming pretreatment on dioxins emission*. Pages 143-153.

Co-treating municipal solid waste incineration fly ash (MSWI-FA) in high-temperature iron ore sintering process is winning great concern. Most of the previous studies were about the co-treatment of raw MSWI-FA (without water washing) in sintering process. Although the content of dioxins in MSWI-FA was reduced, the high chlorine content promoted the secondary synthesis of dioxins and had a negative impact on the quality of sinter. This investigation focused on the emission characteristics and regulation approach of dioxins as co-treating MSWI-FA. The results showed that when MSWI-FA was added without pretreatment, the emission concentration of dioxins in sintering flue gas reached 4.28 ng I-TEQ/Nm³ . After water-washing pretreatment, the chlorine in MSWI-FA was significantly reduced, which inhibited the synthesis of dioxins via de novo reaction. The dioxins decreased significantly to 1.44 ng I-TEQ/Nm³ . Based on the washing pretreatment, the MSWI-FA was further prepared into lumps, which inhibited the dispersion of Cl-containing MSWI-FA particles in mixtures and reduced the active sites of dioxins synthesis, thereby hindering the dioxin synthesis path. The emission concentration of dioxins in sintering flue gas was further reduced from 1.44 ng I-TEQ/Nm³ to 1.15 ng I-TEQ/Nm³ . Adding 0.5% water-washed fly ash lumps had little effect on sintering indexes and dioxins concentration in flue gas. The research results laid a certain foundation for the large-scaly recycling of MSWI-FA.

- **Keywords:** MSWI-FA; Iron ore sintering; PCDD/Fs; Water washing; Roll forming

Shuronjit Kumar Sarker, Warren Bruckard, Nawshad Haque, Rajeev Roychand, Muhammed Bhuiyan, Biplob Kumar Pramanik.

***Characterization of a carbonatite-derived mining tailing for the assessment of rare earth potential*. Pages 154-162.**

Depletion of high-grade deposits of rare earth elements (REEs) has led to increased interest in reprocessing mining tailing, particularly from carbonatite-related deposits. This is because most of the world's REEs are produced from such deposits. The objective of this study was to physically, geochemically, and mineralogically characterize a carbonatite-related tailing from an Australian mine site to assess the REEs recovery potential. The tailing sample sourced from the mine site was analyzed by dry screening, laser particle size analysis, X-ray fluorescence (XRF), X-ray diffraction (XRD), Inductively Coupled Plasma Mass Spectrometry, and Scanning Electron Microscopy-Energy Dispersive Spectroscopy (SEM-EDS). The results revealed that tailing consisted of mainly fine particles with 50 wt% below 61 μm. The geochemical results showed that the tailing consisted mainly of iron (Fe), and REE accounted for over 50% and 9% of the mass, respectively. The identification of major mineral phases by XRD followed by verification by SEM-EDS found monazite and florencite were the main REE-bearing minerals. The main gangue mineral is identified as goethite. The metallurgical balance showed that over 70% of the mass, REE, and Fe were concentrated in finer particle fractions below 63 μm. The SEM-EDS-based mineral liberation analysis found that REE-minerals were primarily associated with goethite and were locked within the latter in larger particle sizes over 100 μm. However, the smaller (<50 μm) REE-mineral grains were mostly liberated. The findings of this study suggest that light grinding of the particle fractions above 63 μm would potentially liberate the locked REE-minerals and subsequent separation by gravity, magnetic, and flotation processes can be tested to make REE concentrate. Because the sample is fine-grained, direct hydrometallurgical processing could potentially be effective to recover REE from this tailing.

- **Keywords:** Critical mineral; Mining tailing; Rare earth elements; Recovery

Xiaotian Bi, Deyang Wu, Daoxiong Xie, Huawei Ye, Jinsong Zhao. *Large-scale chemical process causal discovery from big data with transformer-based deep learning*. Pages 163-177.

Fault diagnosis is critical for ensuring safe and stable chemical production. Correct identification of causal relationships among variables in large-scale chemical processes is a prerequisite for analyzing the root causes and propagation paths of faults. However, chemical process big data often exhibit nonlinearity and nonstationarity, and contain various forms of noise, rendering conventional causal discovery methods vulnerable. In this paper, a novel causal discovery method based on the causality-gated time series Transformer (CGTST) is proposed to address this challenge. By performing time series prediction using the Transformer-based model on the target variable, CGTST measures the causal strength by assessing the contribution of each variable to the prediction through the causality gate structure. Furthermore, a causal validation method based on permutation feature importance is proposed to eliminate spurious causal relationships and ensure robust results. To enhance the performance of causal discovery on nonlinear and nonstationary chemical process data, ensemble empirical mode decomposition is employed to reduce noise. The CGTST-based method is validated on three case studies: a continuous stirred-tank reactor, the Tennessee Eastman process, and a real-world continuous catalytic reforming process. Our findings demonstrate that the proposed method outperforms conventional causal discovery methods and holds promising prospects for industrial applications.

- **Keywords:** Causal discovery; Deep learning; Chemical process; Industrial big data; Multivariate time series prediction

Jian Zhai, Xin Chen, Hongfei Xie, Xiaoqing Sun, Mingyang Hu, Mingyan Dang, Ping Zhao, Yuliang Liu. *Energy-saving heat pump-assisted extractive-azeotropic dividing wall column with heat exchanger network for separating acetonitrile and water: A techno-economic and inherent safety investigation*. Pages 178-190.

In the present paper, a new extractive-azeotropic dividing wall column configuration is designed to recover acetonitrile from wastewater instead of the conventional two-column process. Although the performance of energetic and economic savings is enhanced in the dividing wall column, it is still characterised by high energy consumption. To this end, a methodical framework for designing energy-efficient intensified dividing wall columns is developed to gradually reduce the need for utilities. Results indicate that the reboilers of the extractive-azeotropic dividing wall column can be entirely replaced by the applications of vapour recompressed heat pump and heat exchanger network, which comprehensively improves the energy-saving performance. A multi-criteria evaluation of process sustainability, including energy consumption, total cost, environmental performance, energy efficiency, and inherent safety analysis, is performed among the designs. Results show that the heat-integrated extractive-azeotropic dividing wall column process is inherently safer than the conventional two-column process and reduces at most 51.95%, 89.96%, and 63.58% in total annual cost, CO2 emissions, and total energy consumption, respectively.

- **Keywords:** Azeotrope; Extractive-azeotropic dividing wall column; Heat pump; Inherent safety analysis; Energy saving

Fei Gao, Wenjiang Liu, Xu Mu, Wenhao Bi, An Zhang. *Dependence assessment in human reliability analysis using the 2-tuple linguistic information and DEMATEL method*. Pages 191-201.

Human reliability analysis (HRA), which is to analyze human contribution to system risk, is an effective way to model and assess human errors. Dependence assessment among human errors is an essential part of HRA, which often depends on the judgments of experts. As real-world problems often involve many complex factors, the judgments provided by the experts are often linguistic terms, even under uncertainty. To this end, by integrating 2-tuple linguistic variables and DEMATEL method, this paper presents a novel way to assess the dependence among human actions in HRA. In the proposed method, the linguistic judgments of the experts are modeled using 2-tuple linguistic variables, and the weights of the influential factors are determined using DEMATEL method, furthermore, the conditional human error probability is calculated by aggregating the 2-tuples of different influential factors based on the 2-tuple weighted average operator, where a novel weight calculation method is developed to determine the weights of different experts. Finally, a case study is presented to demonstrate the effectiveness and reliability of the proposed method. By adopting 2-tuple linguistic variables and DEMATEL method, the proposed method could effectively address the uncertainty in the dependence assessment while capturing the relationship among the influential factors.

- **Keywords:** Human reliability analysis; Dependence assessment; 2-tuple linguistic variable; DEMATEL

Jian Zhai, Xiaoqing Sun, Siqi Huang, Hongfei Xie, Xin Chen. *Economic, thermodynamic, environmental, and inherent safety investigation of heat pump-assisted extractive dividing wall column for separating binary azeotrope*. Pages 202-214.

Inherently safer design during the preliminary design stage is vital to reduce the potential risks and accidents of new process design. So far, little effort has been paid to incorporating inherent safety assessment into the techno-evaluation of heat-integrated extractive dividing wall column processes toward sustainable development. To this end, this paper proposes a systematic methodology for designing the energy-efficient extractive dividing wall column processes by applying heat pump and feed preheating techniques to separate binary azeotrope. The proposed approach gradually recovers the waste heat within the process, and the separation of acetonitrile and water is selected as a case. The results show that the total energy consumption, total annual cost, and the CO2 emissions of heat-integrated extractive dividing wall column processes are significantly reduced compared to conventional design, and the thermodynamic efficiency is simultaneously improved. In the process evaluation stage, the inherent safety analysis is performed regarding the Process Route Index and Process Stream Index. Such indices give insights into process safety performance in terms of the overall process and individual streams. The results of the inherent safety investigation show the intensified extractive dividing wall column by a single heat pump performs better than the dual heat pump-assisted process. This multi-criterion evaluation demonstrates a trade-off between inherent safety performance and energy saving in applying a heat pump system in conjunction with the distillation process.

- **Keywords:** Extractive dividing wall column; Heat pump; Inherently safer design; Energy saving; CO2 emissions

Jyoti Rani, Tapas Tripura, Hariprasad Kodamana, Souvik Chakraborty, Prakash Kumar Tamboli. *Fault detection and isolation using probabilistic wavelet neural operator auto-encoder with application to dynamic processes*. Pages 215-228.

Fault detection and isolation are crucial aspects that need to be considered for the safe and reliable operation of process systems. The modern industrial process frequently employs various sensors to measure multiple process variables. However, complex temporal dependencies and intra-channel, as well as inter-channel correlations in the observed multivariate data pause major challenges during fault detection. In this paper, we present the probabilistic wavelet neural operator auto-encoder (PWNOAE), an operator learning model that aims to learn the distribution of these multivariate process data and apply them for fault detection and isolation. Neural operators are networks that can efficiently learn operator dynamics in addition to function dynamics and therefore have better generalizability compared to other models. The proposed PWNOAE utilizes healthy data for learning the distribution, which is then used as a reference for detecting and isolating faults online. For learning the distribution of multivariate time series, the proposed PWNOAE combines the integral kernel with wavelet transformation in a probabilistic fashion. As wavelets help in the time-frequency localization of time series, PWNOAE exploits them to learn complex time-frequency characteristics underlying the multivariate datasets. The fidelity of the proposed PWNOAE is demonstrated using the Tennessee Eastman benchmark data and industrial data recorded from a pressurized heavy-water nuclear reactor operated by the Nuclear Power Corporation of India. The obtained results demonstrate the proposed method's notable efficacy and success in detecting and isolating faults in the time series data compared to various well-established baselines in the literature.

- **Keywords:** Fault detection; Isolation; Neural operator; Wavelets; Probability distribution; Auto-encoders

Zhongze Bai, Xi Zhuo Jiang, Kai H. Luo. *Impact of oxygen and nitrogen-containing species on performance of NO removal by coal pyrolysis gas*. Pages 229-236.

Coal pyrolysis gas is considered a promising reburn fuel with excellent NO reduction performance because of the present of nitrogen-containing species (HCN and NH3) in the pyrolysis gas. In this study, we explored the effects of oxygen and nitrogen-containing species on NO removal performance with HCN and NH3 by reactive force field (ReaxFF) molecular dynamics (MD) simulations. Results indicate that appropriately reducing O2 concentrations and increasing the amount of nitrogen-containing species can benefit the NO reduction performance by coal pyrolysis gas. In addition, the effects of oxygen and nitrogen-containing species content on the NO removal and mechanisms of NO consumption and N2 formation are illustrated during NO reduction with HCN and NH3, respectively. Finally, based on the simulations results, practical operating strategies are proposed to optimize the NO reduction efficiency. In summary, this study provides new insights into NO reduction performance, which may contribute to optimizing the operating parameters to decrease NOx emissions during coal combustion.

- **Keywords:** NO reduction; Oxygen and nitrogen-containing species; HCN; Reactive force field molecular dynamics

Xinyu Xiong, Kai Gao, Jie Mu, Changquan Ji, Bin Li, Dan Zhang, Yadong Xu, Lifeng Xie. *Experimental study on the explosion destructive ability of magnesium powder/hydrogen hybrids in large space*. Pages 237-248.

During the production of magnesium products, it is easy to accumulate powder, which is very easy to derive hydrogen under humid conditions, forming hybrids explosion system. The effect of powder layer thickness on Pmax and flame development process of unpremixed magnesium powder/hydrogen hybrids was investigated by a 4.5 m3 large-size square device with a weak surface. It was found that the damage intensity caused by the explosion of hybrids was significantly greater than that of single-phase hydrogen, and increased with the increase of powder layer thickness. Compared with hydrogen explosion, with the increase of powder layer thickness in the hybrid system, the hydrogen explosion shock wave would roll up more powder to participate in the reaction. This can significantly increased the explosion pressure, the reaction time and the flame coverage area. Interestingly, the Pmax of hybrid explosion on the weak surface of device was instead larger than that on the closed side. In addition, when the weak surface of the device was destroyed, the shock wave would impact the rolled-up powder outside the device to react with oxygen. The flame release temperature was significantly increased, exceeding hydrogen explosion temperature by nearly 900 ℃, and the area covered by high temperature was larger.

- **Keywords:** Unpremixed hybrid explosion; Large size explosion; Shock wave; Flame development process; Temperature field behavior

Shaocang He, Tianpeng Li, Tingting Shen, Jing Sun, Haoqi Pan, Chenxu Sun, Wenxue Lu, Xuqian Lu, Guiyue Gao, Yuxuan Fan, Runyao Li, Enshan Zhang, Dehai Yu. *Preparation and performance of multi-ionic composite coagulants based on coal gasification coarse slag by one-step acid leaching*. Pages 249-262.

Coal gasification coarse slag (CGCS) is a kind of solid waste generated from coal chemical industry. A series of CGCS based multi-ionic composite coagulants were achieved with one-step acid leaching process, optimizing by HCl concentration and acid leaching time. The results indicated that the optimal Coagulant-3.0 showed a remarkable performances on kaolin simulated wastewater with removal efficiency of 98.0% turbidity, 98.0% NH4-N, and 37.0% CODCr, which were of 91.8%, 77.4% and 69.9% for domestic sewage, respectively. Coagulant-3.0 was further characterized by X-ray Fluorescence Spectrometry (XRF), X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), and Scanning Electron Microscope (SEM). It was found that Coagulant-3.0 was

mainly occupied with Fe, Ca, and Al. The good fitting of the pseudo-second-order kinetic model revealed that the co-existence of multi-ions played a synergistic role in the improvement of coagulation performance. Furthermore, the coagulation mechanisms of charge neutralization, adsorption bridging, and sedimentation netting were basically investigated. The work was unique in developing a novel, cost-effective strategy for the production of coagulants based on the intrinsic constituents of CGCS, and providing a safe and efficient way to dispose of CGCS. Additionally, it is potential to offer an alternative pathway for increasing the additional value of the coal chemical industry.

- **Keywords:** Solid waste reutilization; Coal gasification coarse slag; Multi-ionic composite coagulant; Acid leaching method; Wastewater treatment

Yarui An, Baozhong Ma, Xiang Li, Yongqiang Chen, Chengyan Wang, Baohua Wang, Minglei Gao, Guosheng Feng. *A review on the roasting-assisted leaching and recovery of V from vanadium slag*. Pages 263-276.

Vanadium (V) is widely used and is an important strategic resource due to its superior physicochemical properties. Securing the sustainability of vanadium production is crucial due to the rising global demand for the metal. The primary raw material used in vanadium extraction is vanadium slag, which is produced during the smelting of vanadium titanomagnetite (VTM). Resources and the environment both benefit from the recovery of vanadium resources from vanadium slag. This review summarizes the sources and characteristics of vanadium slag, and comprehensively compares and discusses various treatment methods of vanadium slag, including roasting, leaching, precipitation and strengthened vanadium extraction process. Finally, the prospects and challenges of recovering vanadium from slag are assessed. Literature review shows that the roasting assisted leaching process is the most effective way to extract vanadium from vanadium slag. Some promising methods offer the advantages of high selectivity and environmental friendliness and deserve further research in this field in the future. The purpose of this paper is to provide some reasonable development directions for a completely harmless treatment of vanadium slag.

- **Keywords:** Vanadium slag; Roasting; Leaching; Recovery; Resource utilization

Bruno Gambalonga, João Lucas Nicolini, Jordana Mariot Inocente, Claus Tröger Pich, Elídio Angioletto, Fabiano Raupp Pereira, Oscar Rubem Klegues Montedo, Sabrina Arcaro. *Valorization of waste foundry sand aggregates in hot-mix asphalt*. Pages 277-288.

Metal smelting generates a significant volume of industrial solid waste foundry sand (WFS). Although several standards and studies have established practices and requirements for its use, a large portion of the disposed WFS goes to industrial landfills. This study aims to evaluate the value of WFS as an aggregate in hot-mix asphalt mixtures (HMA) using systematic criteria for classification, potentialities, waste generated and applicability. To this end, molding sand (MS) and fine dust of exhaustion (FDE) were characterized, to identify their potential for application as aggregates in asphalt mass. Different contents of MS, FDE, and Blend (BL) were studied according to the normative granulometric ranges of aggregates for HMA. Samples were obtained via the Marshall method to verify important properties for the asphalt mix. Ecotoxicity tests were conducted. The results showed that a composition containing 10 wt% of BL presented an air void volume of 3.3%, a stability of 658 kgf, creep of 2.5 mm, and an indirect tensile strength of 0.93 MPa. From a technical and environmental perspective, a 10 wt% BL content was suitable for recovery into HMA. Lower amounts BL yielded results outside the normative limits. WFS can be recovered and applied as a raw material in HMA.

- **Keywords:** Solid waste; Hot-mix asphalt concrete; Circular economy; Waste foundry sand

Hao-Feng Lin, Ibrahim B. Mansir, Hawzhen Fateh M. Ameen, A. CHERIF, Abdulkareem Abdulwahab, Mahidzal Dahari, Haitao Lin, Ayman A. Aly, Samia Nasr. *Economic, environmental and multi objective optimization of a clean tri-generation system based co-firing of natural gas and biomass: An emergy evaluation*. Pages 289-303.

There is a recognized need for developing the novel clean systems to solve the environmental and energy issues. In this regard, a novel tri-generation system of power, cooling and freshwater triggered by was developed. Emergy analysis was utilized for simultaneously evaluation of system from economic and environmental viewpoints. The effects of gasification temperature, combustion temperature and natural gas contribution in the input fuel to the supercritical carbon dioxide Brayton cycle were studied on system performance. Environmental loading ratio, Emergy sustainability index, Emergy investment ratio, Renewability scale, Emergy yield ratio and energy efficiency were considered as system performance indicators. Response surface methodology was utilized for four-objective optimization of the system performance. The results showed that natural gas contribution in the input fuel was the most effective parameter on system energy efficiency and increasing natural gas contribution in the input fuel resulted in improving the system energy efficiency. Maximization of Emergy sustainability index, minimization of Environmental loading ratio, minimization of Emergy investment ratio and maximization of energy efficiency were considered as the targets of the multi-objection optimization. The findings revealed that natural gas contribution in the input fuel of 1, gasification temperature of 1000 °C and combustion temperature of 1403 °C were the optimum conditions. Response surface methodology efficiently predicted the optimum outputs with errors smaller than 5%.

- **Keywords:** Biomass gasification; Emergy; Multi-objective optimization; Tri-generation system

Sinda Rebello, Huy Truong-Ba, Michael E. Cholette. *Degradation modelling and lifetime assessment for boiler waterwall with incomplete inspection data*. Pages 304-316.

Thermal fatigue cracking is a common problem for boiler waterwall tubes in power plants, resulting the risk of unscheduled plant shutdown. Developing an effective degradation model to predict the future condition of waterwall tubes is vital to assess boiler remaining life. Even though many numerical studies are available in the literature for understanding the physical mechanism (thermal fatigue cracking), the development of predictive models for future risks that can inform decision making are limited. One of the key impediments for developing predictive models is the lack of data. In the case of boiler critical subsystems, very few failures (if any) are recorded in its history. In addition, the number of inspections is limited due to access difficulties. Thus, in many practical cases, the condition data available for degradation modelling is sparse with both infrequent and (spatially) incomplete inspections. This paper presents the development of a stochastic degradation model prediction of thermal fatigue cracking severity in a boiler waterwall when the data is limited. The time evolution of the condition indicator for each waterwall tube is modelled using Markov Models and Bayesian identification algorithms are used to tractably address the large amount of missing data. The methodology presented in this paper employs a Markov Chain Monte Carlo (MCMC) scheme to account for the parameter uncertainty in the presence of missing data. Moreover, this paper also incorporates a novel grouping strategy in which the neighbouring components are grouped to tackle the problem of (spatial) data sparsity. The degradation modelling and prediction tools developed in this paper will support renewal decision making by using available onsite asset data and knowledge. A real-world case study of a boiler waterwall operating in an Australian power industry is also presented. It is found that the waterwall

degradation appears to be slowing, but an additional inspection is recommended to confirm the trend.

- **Keywords:** Bayesian estimation; Boiler waterwall; Degradation modelling; Markov models; MCMC; Missing data

SU Zhanguo, Wu Zhang, Abdulkareem Abdulwahab, S. Saleem, Yuzhong Yao, Ahmed Deifalla, Mohammad Taghavi. *Comparison of gasoline and hydrogen pathways in order to reduce the environmental hazards of a solar-hydrogen refueling station: Evaluation based on life cycle cost and Well-To-Wheel models*. Pages 317-331.

Today, due to increasing concerns about the use of fossil fuels, renewables have been introduced as a popular, efficient and green alternative. Since the transportation sector is one of the most important energy consumers, attention has been directed to the management of this energy consuming sector. It was proven that the development of electric-hydrogen vehicles can significantly reduce environmental concerns and dependence on fossil fuels in the transportation sector. However, improving the infrastructure of hydrogen refueling stations (HRSs) due to the high cost of hydrogen requires more and detailed works. In this article, the conceptual design and economic evaluation of an on-site HRS based on a photovoltaic (PV)-based solar unit coupled with the power grid has been developed and evaluated under various parameters and scenarios. The planned HRS is also comprised of a water electrolysis process (employing a polymer electrolyte membrane (PEM) electrolyzer unit), and hydrogen storage and dispenser. In the developed economic assessment, the levelized cost of hydrogen (LCOH) is calculated and discussed for different scenarios and plans based on the different size of the HRS and energy management approaches. The development of such refueling stations in cities can be an effective direction to achieve sustainable development. In addition, in order to increase believability, globalization and improve economic sustainability, an economic incentive approach based on Well-To-Wheel assessment (WTWA) and life cycle cost assessment (LCCA) was developed. The developed incentive strategy can lead to a decrease in the value of LCOH. A comprehensive comparison between hydrogen and gasoline refueling pathways is also provided. The outcomes indicated that, by applying the proposed economic incentives, the values of LCOH can be reduced by almost 15.5% and 2.98%, respectively, for discounted payback period s of 8 and 10 years. It was also found that, the WTWA index for the gasoline pathway is almost 33.8% higher compared to the hydrogen pathway. In addition, when the participation percentage of the PV-based solar unit is assumed to be 50% and 75%, the value of the WTWA index of the hydrogen pathway is reduced by approximately 25.3% and 62.8% compared to the gasoline pathway.

- **Keywords:** Hydrogen refueling station; Gasoline pathway; Hydrogen pathway; Solar energy; Life cycle cost; Well-to-wheel

Qichao Zhou, Jian Liu, Li Liu. *Fast prediction of mine flow field based on convolution neural network*. Pages 332-343.

Accurately describing the flow state of mine gas is the basis for the prevention and control of mine dust and toxic gases, computational fluid dynamics (CFD) method is often used to solve mine flow field, but CFD method is usually an iterative process with high calculation cost, time-consuming and high memory requirements. In order to realize the fast solution of mine flow field, a prediction model of mine flow field based on convolutional neural network (CNN) is proposed. The geometry flow field simulated by lattice Boltzmann method (LBM) is used as the training data. CNN is used to extract the basic characteristics of the flow field in the training data, establish the mapping relationship between the geometric boundary and the flow field, and quickly predict the

mine flow field. The simulation experiment and the particle image velocimetry (PIV) test experiment of the air window flow field were carried out respectively. In LBM simulation experiment, the average values of mean square error (MSE), mean absolute error (MAE), R2, explained variance score (EVC), Pearson correlation coefficient (PCC) and cosine similarity between CNN predicted values and LBM simulated values of 10 groups of test samples are 0.2633, 0.2449, 0.9595, 0.9697, 0.9827, 0.9933, respectively. It shows that the accuracy of CNN flow field prediction model is similar to that of LBM simulation, and the computational speed of CNN model is increased by three orders of magnitude compared with LBM simulation. In PIV test experiment, the predicted values of CNN model are basically consistent with the PIV experiment results, no matter the velocity distribution of a section or the flow trend of the overall flow field. The LBM simulation experiment and PIV test experiment strongly prove the reliability and generalization ability of CNN model for predicting mine flow field.

- **Keywords:** CNN; Flow field prediction; LBM; PIV; Air window flow field

Chi Zhang, Liting Hao, Hanchen Miao, Jiayu Chen, Tian Yuan, Zhongfang Lei, Zhenya Zhang, Motoo Utsumi, Tomoaki Itayama, Takeshi Miura, Ikko Ihara, Hideaki Maseda, Salma Tabassum, Kazuya Shimizu. Emergence of multidrug-resistant *Acinetobacter baumannii under fluctuating levofloxacin concentration and its control by chlorine and UV disinfection*. Pages 344-353.

Although wastewater treatment plants are considered hotspots for the spread of antibiotic-resistant bacteria (ARB) and antibiotic-resistant genes (ARGs), few studies have explored the mechanisms underlying the emergence of multidrug-resistance. Using four sequencing batch reactors under fluctuating concentrations of levofloxacin (LVX), we isolated 440 isolates, which were identified based on the sequence of the 16 S rRNA gene and growth at 37 ºC, focusing on potential human pathogens. We then evaluated the multidrug-resistance of 62% of these isolates by determining the minimum inhibition concentration (MIC) of erythromycin, tetracycline, chloramphenicol, and LVX in the emergence of ARB. The average MIC was increased more than 100-fold in the first exposure, whereas did not show the same response after re-exposure due to different LVX concentrations between the 2 conditions. We identified 33 Acinetobacter baumannii isolates that emerged only during re-exposure, especially in R-2 and R-3, in which the LVX concentration was changed from 4 and 16 mg/L, respectively, to 128 mg/L. Moreover, we assessed the disinfection efficiency of chlorine/UV treatment against pathogenic ARB. The growth of multidrug-resistant A. baumannii isolates was decreased by 0.9–7.4 log10 following disinfection treatment with > 0.5 mg /L Cl2 or > 30 min UV irradiation.

- **Keywords:** Acinetobacter baumannii; Human pathogen; Levofloxacin; Multidrug-resistance; Sequencing batch reactor

Jirui Chen, Zenan Zhou, Yu Miao, Huan Liu, Wentao Huang, Yifan Chen, Lijian Jia, Wenbiao Zhang, Jingda Huang. *Preparation of CS@BAC composite aerogel with excellent flame-retardant performance, good filtration for PM2.5 and strong adsorption for formaldehyde*. Pages 354-365.

At present, it is still a challenge to prepare an air filtration material with high filter, low pressure drop and good environmental protection. In this study, a porous material with good filtration capacity for PM2.5 and excellent adsorption for harmful gases was developed. Chitosan (CS) was used as the frame matrix, and bamboo activated carbon (BAC) as the functional particles and methyl trimethoxylsilane (MTMS) as the hydrophobic modifier were introduced to the CS system, followed by freeze-dry to

achieve the aerogel sheet with high porosity, flame retardant and hydrophobicity. The resulted CS@BAC composite aerogel showed excellent removal ability for both PM2.5 and formaldehyde in the filtration rate of 94.2% for PM2.5 and the formaldehyde adsorption amount of 61.6 mg/g, which was benefited from the dual removal system, the 3D network structure of the CS based aerogel formed during freeze-dry and the high surface area of BAC itself. In addition, the aerogel displayed outstanding flame-retardant property and its total heat release rate (THR) and maximum heat release rate (PHRR) were only 5.30 kJ/g and 28.2 W/g, respectively, the loss on ignition (LOI) value reaching 33.8%. At the same time, after the modification of MTMS, the aerogel realized the transformation from hydrophilic to hydrophobic, which could be used repeatedly.

- **Keywords:** Chitosan; Bamboo activated carbon; Aerogel; PM2.5; Formaldehyde; Flame retardant

Xiaochuan Xu, Xiaowei Gu, Qing Wang, Yunqi Zhao, Zhenguo Zhu, Fengdan Wang, Zaolin Zhang. *Ultimate pit optimization with environmental problem for open-pit coal mine*. Pages 366-372.

Open pit mining is an effective way to extract valuable minerals from the earth's crust and generate significant profits for mining companies, however it also causes significant environmental harm to vast tracts of land and the surrounding ecosystems. However, the maximization of economic benefits is still the overall objective of optimizing open pit mine design, while environmental issues have been ignored in attempts to achieve more sustainable mine development. Therefore, estimating ecological costs of mining and considering such costs in the mine design process is an important step towards reducing ecological consequences at the design stage. The aim of the study is to calculate the ecological costs of open-pit coal mining and analyze how these costs affect the ultimate pit delineate. The ecological costs associated with coal mining are calculated according to the carbon emissons from energy consumption and the scope of grassland destroyed by resource extraction. There are three key components of ecological cost that have been identified: ecological service value loss, reclamation cost, and carbon emission cost. Necessary equations are provided for estimating these costs. An iterative optimization algorithm is described for ultimate pit optimization in coal deposits with near-horizontal coal seams. A case study is presented in which the ultimate pits are optimized by both with and without considering ecological costs, and compared to prove the impact of ecological costs on the ultimate pit design.

- **Keywords:** Ecological cost; Open-pit coal mining; Ultimate pit optimization; Floating cone exclusion method; Iterative optimization algorithm

Yuchen Jiang, Chao Li, Lijun Zhang, Mengjiao Fan, Shu Zhang, Wenran Gao, Bin Li, Shuang Wang, Xun Hu. *Pyrolysis of banana peel with microwave and furnace as the heating sources: The distinct impacts on evolution of the pyrolytic products*. Pages 373-383.

Microwave pyrolysis features with different heating mechanisms and heat transfer directions from traditional pyrolysis with furnace heating, which might impact evolution of volatiles and nature of biochar in varied ways. This was investigated in this study by pyrolysis of wet and dried banana peel with microwave heating and furnace heating at 400 and 600 °C in a fixed-bed reactor. The results showed that microwave pyrolysis could drastically promote gasification of volatiles to form significantly more gases like H2 via dehydrogenation and CO via cracking and decarbonylation. This was especially evident in the pyrolysis of wet banana peel with abundant water as the heat transfer medium. The dominance of cracking/gasification of volatiles in microwave pyrolysis was due to the rapid heating and the minimized heat transfer limitation, which suppressed the secondary condensation and thus diminished the formation of bio-oil and biochar.

Microwave pyrolysis also favored the cracking of the cellulose/hemicellulose-derived aliphatic organics via cracking but promoted the formation of phenolics via cracking of lignin in banana peel. Moreover, the excessive cracking reactions in the microwave pyrolysis led to the biochar of more excellent thermal stability, lower abundance of oxygen-containing functionalities like CO and more rugged morphology than that with furnace heating source.

- **Keywords:** Microwave pyrolysis; Banana peel; Biochar; Bio-oil; Heat transfer

Ahmed Hamdy El-Kady, Syeda Halim, Mahmoud M. El-Halwagi, Faisal Khan. *Analysis of safety and security challenges and opportunities related to cyber-physical systems*. Pages 384-413.

A cyber-physical system (CPS) is an interconnected physical system that can be monitored, controlled, and operated remotely. A systems-based analysis of CPS is critical for enhancing operational safety and security. Such analysis is particularly important in light of the evolving Fourth Industrial Revolution (Industry 4.0) which is largely driven by CPS, Internet of Things (IoT), algorithmic systems, automation, and smart manufacturing. As a result of industries' and societies' growing dependence on CPSs, their safe and secure applications need to be scrutinized to avoid any threats or harm to processes and human lives. In order to achieve this target, the current work analyzes the literature to investigate challenges and opportunities present in the CPSs. The analysis attempts to answer the following Research Questions (RQs): (RQ1) What are the prominent trends in the field of safety and security of CPSs? (RQ2) What are the opportunities in Industry 4.0 technologies related to safety? (RQ3) What characteristics of CPSs are likely to cause safety and security issues? (RQ4) What are the emerging safety and security issues introduced by CPSs? (RQ5) How were these issues addressed in the literature? CPSs can address some traditional safety issues due to characteristics like high efficiency and control. However, a CPS is challenged by heterogeneity, dependencies, complexity, unattended nature, increased machine intelligence, autonomous reconfiguration, and uncertainties. Safety and security challenges include opaque system failure, complex socio-technical system, human-machine interface, cyber-physical attacks, unsecured remote configuration, lack of standards, and resilience. The paper is structured under the following key headings: bibliometric results, opportunities from Industry 4.0 technologies, issues introduced by Industry 4.0 technologies, literature proposed solutions, and research challenges. Based on the assessment of about 900 relevant publications extracted from two databases (Web of Science (WoS) Core Collection and Engineering village (EV)), the documents were categorized into eight major divisions: (i) Safety Opportunities, (ii) Hazardous Characteristics, (iii) Fault Occurrence, (iv) Cyber-physical attacks, (v) Human factors, (vi) occupational Health and safety, (vii) standards, and (viii) Reliability and resiliency. Proactive strategies were classified under four options: identification, evaluation, prevention, and management. The paper also raises some research needs and unanswered questions that require further analysis to address how security and safety mechanisms can introduce more complexity in the system that can lead to new risks. The paper concludes by emphasizing digital process safety as part of the engineering curriculum to address the process industry's need for digital solutions and to make process safety learning a conscious choice.

- **Keywords:** Cyber-physical systems; Process safety and security; Process risk management; Process failure analysis; Process fault diagnosis; Process automation

Seyed Mohammad Seyed Mahmoudi, Ehsan Gholamian, Nima Ghasemzadeh. *Recurrent machine learning based optimization of an*

***enhanced fuel cell in an efficient energy system: Proposal, and techno-environmental analysis*. Pages 414-425.**

Real hybrid energy systems based on developing fuel cell (FC) technology are promising in addressing energy and environmental problems. Before looking at the research investigations, the earlier review studies are briefly examined to spot any gaps in the literature. In the present study, a novel scheme of fuel cells is introduced with higher efficiency and compatibility. The exhaust gases are then introduced to the transcritical carbon dioxide cycle for the production of more power and to extract heat from the intercoolers. The system is analyzed from the multiple objective functions aspect, and the net present value method is occupied for determining the system's payback period. The important design conditions are then put to the test to seek their effect on the overall system. The genetic algorithm is applied for the sake of optimization, and the efficiency is maximized while minimization of environmental impact and the cost of the system. The results indicate that maximum ηII and minimum of LCOP and ζ at the ideal point which equals to 73.8%, 0.24 $/MWh and 0.07 kg/kWh, can be reached correspondingly. Also, by changing the selling price of electricity from 0.19 $/kWh to 0.22 $/kWh, the net present value and the payback period reach 1329000 $ and 6.24 years, respectively.

- **Keywords:** Optimization; S-CO2; SOFC; Machine learning; Techno-economic; Environmental analysis

Alyne Moraes Costa, Marllon Robert dos Santos Valentim, Diogo José Menezes de Azevedo, Bianca Ramalho Quintaes, Sarah Dario Alves Daflon, Juacyara Carbonelli Campos. *Evaluation of the main pollutants present in Brazilian landfill leachates using ecotoxicity assays*. Pages 426-436.

The present study investigated the acute toxic effects caused by the main pollutants found in landfill leachates: total ammonia nitrogen (TAN), alkalinity, and humic substances (HS) for the test organisms Vibrio fischeri, Danio rerio, Daphnia similis, and Artemia sp. The leachates were obtained from two Brazilian landfills with different ages and operating modes. Air stripping and membrane filtration treatability experiments were performed to remove pollutants from the leachate. The results showed high toxicity of the raw leachate from both landfills for the studied organisms. In the individual treatments, air stripping achieved TAN and alkalinity removal efficiencies > 99%, and the membrane filtration treatment achieved HS removal efficiencies > 98%. Compared to the individual treatments, the combination of treatments resulted in the most significant reductions in leachate toxicity from both landfills for all test organisms studied. The principal component analysis showed a strong correlation between COD or HS parameters and the toxicity of V. fischeri and strong correlations between TAN and the toxicity of D. rerio, D. similis, and Artemia sp. Finally, this study highlights the application of a treatment route to remove acute toxicity from complex effluents, such as landfill leachate, to avoid potential environmental hazards to the aquatic ecosystem.

- **Keywords:** Landfill leachate; Acute toxicity; Vibrio fischeri; Membrane filtration; Humic substances; Ammonia nitrogen

Yunfeng Zhu, Bo Li, Yonggang Wei, Shiwei Zhou, Hua Wang. *Recycling potential of waste printed circuit boards using pyrolysis: Status quo and perspectives*. Pages 437-451.

Resource shortages and metal demand continuously increase, and the massive quantities of waste printed circuit boards (WPCB) generated make resource recycling and environmental sustainability necessary paths. Pyrolysis is a practicable and promising

pathway to lessen the environmental burden through the conversion of WPCB into high value-added products. In this study, the characteristics of WPCB are first analyzed, and the types of pyrolysis reactors for WPCB and the characteristics of pyrolysis products are introduced. Then, we summarize and compare the conventional and advanced pyrolysis technologies applied to the treatment of WPCB for the scientific management and sustainable recovery of WPCB. In addition, we present an overview of possible pathways for the subsequent treatment of pyrolysis products. Furthermore, we discuss the prospects of WPCB pyrolysis, emphasize the imperatives and significance of establishing a circular economy for WPCB, and discuss the economic feasibility and future challenges of WPCB pyrolysis. Pyrolysis of WPCB has been proven at the laboratory scale; however, more effort and time are required for industrialization.

- **Keywords:** Waste printed circuit boards; Pyrolysis; Sustainable recycling; Resource utilization

Tengfei Zhou, Jinhua Ou, Tao Xu, Yihui Zhou, Xiping Lei, Bonian Hu, Xueyuan Zhang, Gang Yu. *The process and mechanism of pulse electrolytic oxidation of ciprofloxacin antibiotic in wastewater on boron-doped diamonds*. Pages 452-460.

A novel process and method for treating ciprofloxacin (CIP) antibiotic wastewater using pulsed electrooxidation at boron-doped diamond (BDD) electrodes have been developed to address the issues of low efficiency and high energy consumption associated with traditional electrochemical oxidation methods. The effects of pulsed direct current (PDC), pulsed alternating current (PAC), and direct current (DC) on chemical oxygen demand (COD) removal were studied. It was found that complete degradation of CIP could be achieved within 45 min using PAC. COD removal reached 92.4% after 90 min of PAC electrooxidation for 90 mg·dm−3 CIP wastewater under optimized conditions of current density (j) = 30 mA·cm−2, initial pH (pH0) = 3, sodium sulfate concentration (c(Na2SO4)) = 50 mmol·dm−3, and frequency (f) = 100 Hz. The electrical energy consumption (EEC) was found to be 35 W·h·dm−3. The CIP degradation followed a quasi-first order kinetic law. The degradation pathway was found to involve hydroxylation of the quinolone moiety, cleavage of the piperazine ring, and fluorine substitution (OH/F substitution). The results showed that PAC electrochemical oxidation at all-BDD electrodes exhibited the highest removal efficiency and lowest EEC for CIP removal. This study provides a novel and effective approach for the efficient treatment of CIP antibiotic wastewater using bidirectional pulse current at all-BDD electrodes.

- **Keywords:** Pulse electrooxidation; Boron-doped diamond electrode; Ciprofloxacin; Process optimization; Degradation mechanism

Zeqi Wang, Zhanguo Su, Vishal Goyal, N. Bharath Kumar, Mahidzal Dahari, Abdulkareem Abdulwahab, A.M. Algelany, Fatma Aouaini, Husam Rajab, H. Elhosiny Ali. *Optimization and evaluation of a municipal solid waste-to-energy system using taguchi technique in a tri-generation system based on gas turbine with air and steam agents*. Pages 461-471.

There is a recognized need for treating the municipal solid waste which causes serious environmental problems. There has been substantial research undertaken on the role of municipal solid waste in integrated energy systems. However, the contribution of Taguchi technique has received little attention within the field of municipal solid waste-to-energy systems. This study set out to examine the capability of utilizing the Taguchi technique in optimization and evaluation of a tri-generation system based on gas turbine. L25 orthogonal array of Taguchi technique has been utilized considering compression factor of compressor, maximum temperature of input stream to the gas turbine, and municipal solid waste fed to the combustion chamber as the input variables. Electrical power of the

system, heating air and water capacities of the system, system efficiency, and normalized emission have been also considered as the tri-generation system performance indicators. The air-based system operates optimally at compression ratio of 10, maximum temperature of 900 °C, and fed MSW of 1 mol/s while compression factor of 15, maximum temperature of 1000 °C, and fed MSW of 1.2 mol/s are optimum conditions for steam-based system. Overall, air-based system operates better than steam-based system with electrical power of 317.6 kW, heating air capacity of 678.4 m3/min, heating water capacity of 288.7 L/min, efficiency of 79.3%, and normalized emission of 8.58 g/kW.min.

- **Keywords:** Waste-to-energy; Municipal solid waste; Taguchi; Optimization; Analysis of variance

Yuchuan Yang, Jiantao Lin, Zhengxu Liu, Minghua Liu. *Degradation of tetracycline by peroxydisulfate activation on sludge-derived biochar modified with tannin extract*. Pages 472-484.

In this study, the waste sludge was modified by tannin extract, and the modified material Tannin Extract-Sludge Derived Biochar (TE-SDBC) was prepared by high-temperature pyrolysis at 700 degrees , while tannin extract dosage was 3.17 g, pH value was 7.69. TE-SDBC was used to activate peroxydisulfate (PDS) for the degradation of tetracycline(TC). The sludge-based biochar was characterized by ATR-FT-IR spectroscopy, BET, SEM, XRD, XPS. The following preparation conditions for TE-SDBC were tannin extract dosage was 3.17 g, pH value was 7.69 and pyrolysis temperature was 717.3 ℃. TE-SDBC had more defect sites and higher pyridinic N content, which was conducive to promote the PDS activation, indicating that TE-SDBC had better catalytic performance. The TE-SDBC obtained optimal conditions were as follows: the initial mass concentration of TC was 20 mg/L, TE-SDBC dosage was 0.15 g/L, PDS dosage was 0.1 g/L, initial pH of pollutant solution was 5.76 and the reaction temperature was 25 ℃. The degradation of TC by TE-SDBC/PDS and SDBC/PDS was explored. After 120 min reaction, the degradation efficiency of TE-SDBC/PDS was 40% higher than that of SDBC/PDS, and the optimization of the conditions indicated that the TE-SDBC/PDS system had a better removal effect on TC degradation. Under the action of reactive oxygen species, the breakage of CC bond happened, the functional groups, i.e., amino, methyl and hydroxyl, were removed, and the ring opening reaction occurred in TC molecule, then the small molecular intermediates were ultimately formed. Finally, the intermediate products were mineralized into CO2, H2O and various inorganic substances.

- **Keywords:** Tannin extract; Sludge; Biochar; Tetracycline; Degradation

Xinyuan Zhan, Yan Wang, Li'ao Wang, Chenxuan Li, Xiaowei Xu, Rui Deng. *Migration, solidification/stabilization mechanism of heavy metal in lightweight ceramisite from co-sintering fly ash and electrolytic manganese residue*. Pages 485-494.

Municipal solid waste incineration (MSWI) fly ash and electrolytic manganese residue, as hazardous waste, were roasted into lightweight ceramisite with coal fly ash. The migration, transformation and stabilization/solidification mechanism of heavy metals during ceramisite formation process was explored. Heavy metals in ceramisite pellet were concentrated and experienced the transportation among solids below 710 ℃, then heavy metals were prone to flue gas in the form of chlorides above 710 ℃, in particular for Pb, Cd and Cu. Heavy metal chlorides depended on the generation of HCl and Cl2, which needs co-existence of silicon oxide and aluminum oxide. Note that gibbs free energy change of copper chlorides generation reaction decreased with temperature, resulting in higher volatilization rate compared with Mn, Zn and Cr. Remained heavy metals in the solid phase like Cu, Zn and Cr were prone to ion-exchange, balance-charge and specific-

adsorb with calcium-bearing minerals (Ca(Mg,Al)(Si,Al)2O6 and (Ca,Fe)SiO3) in ceramisite based on mineral analysis and principle component analysis at 1160 ℃.

- **Keywords:** MSWI fly ash; Ceramisite; Heavy metals; Migration; Transformation

Maryam Safaripour, Ehsan Parandi, Babak Aghel, Ashkan Gouran, Majid Saidi, Hamid Rashidi Nodeh. *Optimization of the microreactor-intensified transesterification process using silver titanium oxide nanoparticles decorated magnetic graphene oxide nanocatalyst*. Pages 495-506.

In the current study, the biodiesel fuel generation from waste cooking oil (WCO) as a low-cost feedstock was performed in a T-shaped microreactor through a transesterification process in the presence of binary metal oxide of silver-titanium oxide nanoparticles doped over magnetic graphene oxide (MGO@TiO2Ag) as a novel catalyst. Scanning electron microscopy (SEM), Transform Infrared Spectroscopy (FTIR), vibrating-sample magnetometer (VSM), Energy-Dispersive X-ray Spectroscopy (EDX), and Powder X-ray diffraction (XRD) were employed to characterize the MGO@TiO2Ag nanocatalyst. The Box-Behnken design (BBD) based on the response surface methodology (RSM) was used to optimize the reaction parameters, including methanol to oil volume ratio (Me/Oil), residence time and catalyst concentration. Following data analysis and optimization of the transesterification reaction, the maximum yield of fatty acid methyl esters (FAMEs) which was equal to 96.54 ± 1.16 %, was achieved at the residence time of 169.15 s, Me/Oil ratio of 2.52, and catalyst concentration of 4.15 wt%. All attributes of the manufactured FAMEs were within the permitted ranges of the ASTM D6751 standard, indicating high quality. The finding of this work demonstrated that employing a microreactor has an influential role in producing FAMEs in the presence of an MGO@TiO2Ag nanocatalyst.

- **Keywords:** Microreactor; Magnetic nanocomposite; Biodiesel; Transesterification; Box-Behnken design

Jitendra Choudhary, Bablu Alawa, Sankar Chakma. *Insight into the kinetics and thermodynamic analyses of co-pyrolysis using advanced isoconversional method and thermogravimetric analysis: A multi-model study of optimization for enhanced fuel properties*. Pages 507-528.

Waste management is quite challenging and it has become a major concern across the globe. The most common wastes are in the form of polymers or plastics that are composed of a mixture of various commodity plastics like PE, PP, PVC, HDPE, LDPE, etc. Pyrolysis is found to be a promising technology for managing wastes as well as converting them into valuable hydrocarbons. The present study investigated to discern the synergism in thermal degradation behavior and to identify the interaction between polymer molecules in co-pyrolysis. The advanced isoconversional model was employed for trustworthy estimation of activation energy as the thermal effects on a reaction deviate the temperature of a sample from the set heating value. The results were also compared with the model-free methods to understand the synergism, reactivity, and thermodynamic system with the progress of the conversion. The activation energy was found to be lowest when the polymers were used in a certain proportion and the synergy effect was more significant when PP content was > 40 % in the mixture. The positive synergetic effect could be attributed to the intermolecular hydrogen transfer from a less stable polymer to a free radical de-propagating chain of the other polymer during thermal degradation. The complex governing thermochemical reaction mechanism was determined using the Criado master plot and the analysis revealed that with increasing PP content in a binary mixture the reaction mechanism shifted from R2 to R3. The high regression coefficient value (R2 > 0.99) in the regenerated TGA profiles signified a good agreement between the theoretical and experimental results. While thermodynamic

analysis showed that the process was endothermic and non-spontaneous in nature. Moreover, the radical reaction during co-pyrolysis of polymers enhances intermolecular hydrogen transfer resulting in the formation of iso-alkane and iso-alkene along with secondary radicals, which undergo β-scission to form alkenes/dienes and short primary radicals. As a result, the enhanced intermolecular hydrogen transfer phenomenon initiates the co-pyrolysis reaction at a relatively lower activation energy compared to individual polymer molecules.

- **Keywords:** Thermogravimetric analysis; Thermodynamic analysis; Co-pyrolysis; Waste plastics; Isoconversional kinetics; Compensation method

Allan Soo, Li Wang, Chen Wang, Ho Kyong Shon. *MachIne learning for nutrient recovery in the smart city circular economy – A review*. Pages 529-557.

Urbanisation is leading to a concentration of growing city populations that contribute significantly to economic growth, while becoming epicentres of waste generation, greenhouse gas emissions, and food consumption. Nutrient smart city circular economy is currently an understudied intersection of growing city populations of food consumers, nutrient recovery technologies, Internet of Things (IoT), and agriculture. Meanwhile, machine learning has exploded with popularity over the years, with many circular economy literatures examining its usefulness in its predictive qualities to support management, optimisation, and recovery of useful resources from organic waste. This review paper examines advancements in machine learning for macronutrient recovery in city organic waste systems for a circular economy. The use of ML will greatly improve the scalability, transparency, productivity and accuracy of nutrient: recovery technologies, logistics, dissemination, and reuse. ML can also be combined with hardware to automate tedious waste separation, recovery and agricultural tasks using drones, hydroponics and satellites. Meanwhile, crop yields, nutrient demand-supply efficiencies, food security, environmental soil monitoring, and prosumer involvement could all increase. However, ML applications for urine, anaerobic digestion and prosumer economics are lacking.

- **Keywords:** Nutrient; Circular economy; Smart city; Machine learning; Internet of things; Sustainability

Ana Ligero, Mónica Calero, Antonio Pérez, Rafael R. Solís, Mario J. Muñoz-Batista, M.Ángeles Martín-Lara. *Low-cost activated carbon from the pyrolysis of post-consumer plastic waste and the application in CO2 capture*. Pages 558-566.

Chemical recycling by pyrolysis of plastic waste has been considered a potential approach. However, little attention has been paid to the reuse of the char residue generated. The preparation of materials from char residue obtained from the pyrolysis process has become an essential task. The purpose of this work is the preparation of activated carbons from the resulting char from the pyrolysis of a dirty and wet mixture of post-consumer plastic waste. The porous materials have been applied to the adsorption of CO2. Both physical and chemical activation methods were investigated to modify the surface texture properties. The properties of the developed activated carbons were characterized by diverse techniques such as elemental and proximate analysis, Fourier Transform Infrared Spectroscopy (FTIR), adsorption-desorption isotherms with N2, and Scanning Electron Microscopy (SEM). Among all synthesized samples, the activated samples prepared by chemical activation with KOH (char: KOH ratio 2:1; surface area, 487.0 m2·g−1) exhibited the highest CO2 adsorption uptake (~49 mg·g−1). The activation temperature was explored within 680–840 ºC. For physical activation, an increase in the activation temperature decreases the adsorption uptake of the samples. For chemical activation, the adsorption increased as activating temperature rise to a

maximum value, subsequently decreasing with further temperature rise. Increasing the amount of the chemical activating agent significantly decreases the adsorption capacities. The best-activated carbon was chosen, and several parameters were investigated on CO2 adsorption, C: KOH mass ratio (6:1–1:4), and adsorption temperature (15–60 °C). The highest adsorption of CO2 achieved was 62.0 mg·g−1 for activated carbon operating at the lower adsorption temperature (15 ºC).

- **Keywords:** Plastic waste; Char pyrolysis; Activated carbon; CO2 adsorption

Yutao Zhang, Ruzhen Zhao, Xiaohuan Zhang, Qifeng Wei, Xiulian Ren, Ziwen Ying. *A novel technology for producing high-purity V2O5 from hazardous vanadium-containing solutions using precipitation and solvent extraction*. Pages 567-578.

In this study, a novel and cleaner production process was developed to remove impurity anions by precipitation and purify vanadium by solvent extraction using an ionic liquid. After optimizing the precipitation process parameters and conducting an orthogonal test, most of the impurity anions were removed. Then, the extraction and stripping process parameters for recovering vanadium (V) in the filtrate were optimized, and the vanadium extraction and stripping efficiency reached more than 99.8% and 99.9%, respectively. The V2O5 product with a purity of over 99.8% was obtained. The extraction mechanism of vanadium (V) with the ionic liquid was investigated in-depth with the slope method and FT-IR analysis. Further, the essence of the extraction process was expounded at the molecular level with molecular electrostatic potential analysis.

- **Keywords:** Vanadium; Precipitation; Solvent extraction; Ionic liquid; Extraction mechanism

Jigang Zhang, Zhiwei Chu, Weihong Liu, Zhaocai Teng, Kuihua Han. *Pilot experimental study on pollutant emission characteristics from co-combustion of coal and spent cathode carbon block*. Pages 579-591.

Spent cathode carbon block (SCCB) is a hazardous waste produced by the electrolytic aluminum industry. Collaborative treatment of the SCCB in pulverized coal boilers is a potentially valuable technology. Pilot experiments were carried out on a 240 t/h pulverized coal boiler and its supporting flue gas treatment measures as a function of the mixing ratio of SCCB to verify the feasibility of coal collaborative disposal of SCCB. The thermal conversion characteristics of fluoride after mixing SCCB with coal were studied. A continuous emission monitoring system was used to monitor the impact on SO2, NOx and particulate matter in real time. The effectiveness of existing flue gas control measures was evaluated, and optimization suggestions of the flue gas control measures were postulated. The content of heavy metals (Hg, Cd, Ni, Pb, As, Se) in solid waste from co-combustion and the physical phase of solid waste were investigated. In addition, the transformation of heavy metals such as Hg, Cd, Ni, Pb, Cr, As and fluoride in defluorination wastewater during flue gas treatment were analyzed. The results show that it is feasible to use a pulverized coal boiler to dispose SCCB. The existing flue gas treatment measures proved to be appropriate, and desulfurization wastewater can achieve the discharge standards. Defluorination gypsum, fly ash and slag are not hazardous waste. When the mixing ratio of SCCB is increased, the existing neutralization and flocculation precipitation processes of the desulfurization wastewater are affected. It is suggested to add Al2O3 for the defluorination process before the desulfurization tower.

- **Keywords:** Spent cathode carbon block; Pulverized coal boiler; Collaborative disposal; Fluoride; Solid waste; Pilot test

Tu Xayachak, Nawshad Haque, Deborah Lau, Raj Parthasarathy, Biplob Kumar Pramanik. *Assessing the environmental footprint of plastic pyrolysis and gasification: A life cycle inventory study*. Pages 592-603.

Chemical recycling is a promising technology that can help alleviate the environmental burdens of plastic waste. This paper developed a comprehensive, scenario-based life cycle assessment (LCA) to quantify the environmental profile of different management options to treat polyethylene (PE) and polypropylene (PP), including landfill, pyrolysis, and gasification. Using a system expansion method and inventory data from various sources, the result showed that the recovery of ethylene and propylene monomers for plastic re-manufacturing, which resembled closed-loop recycling systems, offered the highest environmental benefits. Most notably, fossil fuel depletion, climate change, and human toxicity impacts were 36,761%, 1063%, and 329% lower than those of landfill disposal, respectively. Open-loop recycling scenarios, such as high-value chemical (HVC) and energy recovery from pyrolysis and gasification, were also investigated. Amongst these scenarios, pyrolysis for HVC recovery was the most environmentally favourable, followed by HVC recovery using gasification. Energy recovery scenarios offered limited benefits and had worse results than landfill in terrestrial acidification, freshwater and marine eutrophication impact categories. The main driver of impacts during end-of-life treatment using chemical recycling is the energy consumption needed to achieve appropriate temperature for the necessary reactions to take place. In terms of material consumption, the use of nitrogen gas to purge the reactor is the biggest contributor for pyrolysis whereas zeolite usage accounts for the majority of material impacts for gasification.

- **Keywords:** Life cycle assessment; Plastic waste; Chemical recycling; Gasification; Pyrolysis

Zhuoyue Guo, Canyun Yang, Dongsheng Wang, Hongbin Liu. *A novel deep learning model integrating CNN and GRU to predict particulate matter concentrations.* Pages 604-613.

PM2.5 is a significant environmental pollutant that damages the environment and endangers human health. Precise forecast of PM2.5 concentrations is very important to control air pollution and improve people's life quality. In the subway indoor air quality (IAQ) system, the data collected by telemonitoring systems is frequently lost due to many reasons. A deep learning model called RF-CNN-GRU, which combines random forest (RF), convolutional neural network (CNN) and gated recurrent unit (GRU), is proposed to predict atmospheric PM2.5 concentrations with incomplete original data. The RF-CNN-GRU model employs the RF to fill in missing values in the data and subsequently applies the CNN to extract features from the imputed data. The data is finally sent to the GRU network to train and predict PM2.5 concentrations. Comparing with single CNN, GRU and long short-term memory (LSTM) models, the predictive accuracy of the RF-CNN-GRU model is significantly improved. The RF-CNN-GRU model shows a slight improvement in prediction results when compared to models such as CNN-GRU, RF-CNN, RF-GRU, and RF-LSTM. The findings demonstrate that the RF-CNN-GRU model has excellent accuracy in PM2.5 concentration prediction when the original data is incomplete.

- **Keywords:** Indoor air quality; Deep learning; Random forest; Convolutional neural network; Gated recurrent unit; Concentration prediction

Chunyang Gao, Bing Wang, Xingchun Li, Yuzhu Zhang, Tongxu Qu, Xianyuan Du, Jin Zheng, Jinguo Feng. *Removal of Cr(VI) by hollow micron zero-valent iron in groundwater containing different ions: Mechanisms and mineralized products*. Pages 614-626.

The development of zero-valent iron in-situ reactive zone technology is restricted by the poor mobility and reactivity of zero-valent iron. Hence , hollow micron zero-valent iron (H-mZVI) was prepared through rapid liquid reduction and used to remove Cr(VI) from aqueous solution. Scanning electron microscopy confirmed that H-mZVI had a hollow structure, particle size of approximately 1 μm, and rough surface. X-ray diffraction indicated that H-mZVI was mainly composed of ZVI. Brunauer–Emmett–Teller results showed that H-mZVI had a large specific surface area (25.54 m2/g) and pore volume (0.12 cm3/g). The Cr(VI) removal efficiency of H-mZVI was 6.18 times that of solid micron zero-valent iron (S-mZVI), and the removal reaction conformed to first-order reaction kinetics. Electrochemical test results revealed that the electron transport efficiency was stronger, Fe2+ concentration in aqueous solution was larger, and the decrease in oxidation–reduction potential was more obvious in H-mZVI than in S-mZVI. Desorption experiment and X-ray photoelectron spectroscopy showed that H-mZVI removed Cr(VI) primarily through reduction and secondarily through adsorption. The effects of conventional ions and humic acid (HA) on Cr(VI) removal by H-mZVI were in the order of PO43->HA>NO3->CO32->HCO3->Cl-=Mg2+=Ca2+. The corrosion products and their proportions varied in the presence of different ions.

- **Keywords:** Hollow micron zero valent iron; Cr(VI); Ion types; Mineralisation mechanism

Xingyu Wen, Shixiao Zhong, Wei Sun, Wei Xue, Wenshuai Bai. *Development of an optimal bilayered back propagation neural network (BPNN) to identify thermal behaviors of reactions in isoperibolic semi-batch reactors*. Pages 627-641.

It is very important to identify the thermal behaviors of semi-batch reactors (SBRs) in isoperibolic operating mode. First, a default bilayered back propagation neural network (BPNN) is selected from multiple recognition algorithms to achieve this task, which is suitable for three kinds of reactions with arbitrary reaction orders: homogenous, kinetically−controlled, and diffusion−controlled liquid−liquid heterogeneous reactions. Then, it is further optimized by Bayesian regularization and genetic algorithm (GA). The result shows that the optimal bilayered BPNN undoubtedly has better recognition accuracy and generalization performance. It is found that the accuracy of the two test sets are 98.8% and 100%, respectively. Subsequently, a simple and user-friendly standalone desktop application program (app) is designed to easily use the developed optimal bilayered BPNN. Finally, a case of acetic anhydride hydrolysis reaction with acetic acid solvent is studied to prove the good validity of the bilayered BPNN and the great reliability of the standalone desktop app.

- **Keywords:** Thermal behavior; Isoperibolic SBRs; BPNN; GA; App; Acetic anhydride hydrolysis reaction

Mohammad Shahab-Deljoo, Bijan Medi, Monzure-Khoda Kazi, Mostafa Jafari. *A techno-economic review of gas flaring in Iran and its human and environmental impacts*. Pages 642-665.

Today, managing energy consumption in industries has become a necessity. Flaring the combustible gases is the main source of wasting energy in the oil and gas explorations, refineries, and petrochemical industry. Flaring contributes to the release of large amounts of environmental pollutants, such as CO2, SOx, NOx, and hydrocarbons, as well as other adverse human and environmental effects. In this regard, flaring reduction or recovery of flared gases has become one of the main concerns of the relevant industries. With 17.40 billion cubic meters (BCM) of annual flared gasses, Iran held the third rank among the top most gas flaring countries in 2021. Flaring such an amount of gas signifies a considerable economic loss as well as the emission of large volumes of greenhouse

gasses (GHGs). Air pollution caused by flaring is a long-lasting problem in the oil-rich regions of Iran, while traces of heavy metals have been found in the Zagros ecosystems in the soil and tree leaves. We have also presented the most updated status of flare gas recovery (FGR) projects (AMAK, Kharg NGL, and Siri projects) with some promising results. To analyze the recovery potential of flare gases in Iran, different technologies and decision-making factors have been critically reviewed with the goal of finding the best recovery methods. Based on our study, there are new hopes for investment, particularly from the private sector, despite some resistance in the oil and gas administration. The proximity of Iran's giant petrochemical complexes to the major associated and non-associated gas flaring sites and the feasibility of their utilization as the feedstock signal favorable changes and is a positive outcome of this research. The expected rate of return (ROR) for feedstock production is between 120% and 250% and payback period (PB) between 0.4 and 1.2 years. Due to massive inflation and difficulties in foreign financing and technology transfer, we recommend more straightforward recovery methods despite lower profit. In this regard, apart from feedstock utilization of associated gas, we recommend electricity generation from flare gases for smaller amounts of flaring since the technology is more available and the country is always in shortage of the product (electricity). The ROR and PB for electricity generation are reported to be between 15% and 40% and 2.5–6.5 years, respectively.

- **Keywords:** Gas flaring; Emissions; Flare gas recovery; Environmental impacts, economic

Deepankar Kumar Ashish, Surender Kumar Verma, Minkwan Ju, Himanshu Sharma. *High volume waste foundry sand self-compacting concrete – Transitioning industrial symbiosis*. Pages 666-692.

In light of massive industrialization, Industrial symbiosis has gained traction by most countries to employ wastes of one industry as a resource to another. Waste foundry sand obtained from the metal casting industry is a threat to the environment and the health of living beings due to the presence of organic and inorganic materials. However, this waste can be a resource for the construction industry. Despite its broad application scope, usage of waste foundry sand is highly limited due to inadequate understating of its performance in concrete. It becomes essential to understand the behaviour of waste foundry sand in concrete, more importantly, for accessing a strength-efficient and durable structure. The concrete samples were examined by conducting a number of experiments to investigate ties between strength, durability and microscopic insights. It has been observed that the inclusion of waste foundry sand can improve strength properties at later ages. Particular attention is paid to study the detailed microstructural investigations conducted on the concretes having up to 50% waste foundry sand. In addition, a leaching analysis was performed that revealed an increase in heavy metal concentration with the increasing WFS content. However, its concentration was below the acceptable limit, as evidenced by USEPA. Mineral and compositional characteristics monitored the effect of calcium aluminosilicate in the concrete matrix from early to later ages by X-ray diffraction and energy dispersive spectrometer analysis for the solid constituents of the concrete specimen, respectively. In light of the above, this study reveals that the strength properties of blended SCC were improving at later ages; significant improvement was discovered after 91 days of curing time. The compressive strength results were observed to increase by 16.6% for the specimens containing 40% waste foundry sand relative to control concrete at 91 days. The highest strength properties were achieved at 365 days, with 50% replacement ratios of waste foundry sand. The values for UPV were observed to improve as the curing age increases with the reduction in the rate of carbonation resistance of concrete. The carbonation depth was observed to be less than 1 mm for specimens containing 40% and 50% waste foundry sand for accelerated and atmospheric carbonation at 56 days and 2 years, respectively. The originality of the study relies on the possibility of developing waste foundry sand-self compacting concrete with the maximum utilization of waste foundry sand, achieving the

targeted results. The study showed a good agreement between the waste foundry sand and concrete that creates a ground for the enhanced application of industrial symbiosis.

- **Keywords:** Circular economy; Low-carbon development; Sustainable future; Resources conservations; Microstructure; Leaching

Qun Zhou, Botao Qin, Banghao Zhou, Huixiang Huang. *Effects of surfactant adsorption on the surface functional group contents and polymerization properties of coal dust*. Pages 693-701.

In order to better explain the wetting and polymerization mechanism between surfactant and coal dust, the effects of surfactant adsorption on the surface physicochemical properties of coal dust were investigated based on the infrared spectroscopy, zeta and dust control efficiency experiments. The results showed that compared with nonionic surfactant, anionic surfactant was more easily adsorbed on coal dust surface, while the combination of anionic-nonionic surfactants made surfactant molecules more easily adsorbed on the surface of coal dust, especially compound surfactant (B+D). With the surfactant adsorption increased, the hydrophobic functional group content and absolute potential value of coal dust decreased. For example, the surface potential and hydrophilic functional group content of coal dust adsorbing the compound surfactant (B+D) was enhanced by 43.92%, 165.7% than that of single surfactant (B). Additionally, it was verified that surfactant adsorption capacity could not be used as a critical factor to optimize surfactants applied to enhance the solution wettability. In field tests, the developed compound surfactant (B+D) enhanced respirable dust and total dust control efficiencies by 41.86% and 40.16%, respectively, compared to that of water spray. This study was conducive to choose surfactants to improve coal dust control performance of the aqueous solution.

- **Keywords:** Coal dust; Surfactant adsorption; Functional group content; Polymerization property; Dust control efficiency

Shichao Wu, Tichang Sun, Hongda Xu. *A new way to efficient utilization of eggshell waste: As green dephosphorization agent and accelerator for reduction roasting of high-phosphorus oolitic iron ore*. Pages 702-714.

The cleaning and efficient disposal of eggshell waste presents many challenges. Reduction roasting of high-phosphorus oolitic iron ore (HPOIO) requires the addition of expensive alkali metal compounds to enhance dephosphorization. In this paper, the eggshell waste from the catering industry was used to replace traditional dephosphorization agents, which not only avoided environmental problems caused by mining, but also improved dephosphorization and iron extraction, and reduced production costs. Under suitable conditions, powdery reduced iron (PRI) comprising 93.04% iron and 0.09% phosphorus was produced. PRI is a premium steelmaking feedstock with 93.11% iron recovery. Mechanism research shows that an appropriate eggshell waste dosage inhibited the reduction of apatite in HPOIO, reacted with phosphorus in iron minerals to form apatite, and promoted the metallization of iron. Moreover, compared with blast furnace ironmaking, this process significantly reduced carbon emissions. It provides a new idea for the green utilization of eggshell waste.

- **Keywords:** Eggshell waste; Clean utilization; High-phosphorus oolitic iron ore; Reduction roasting; Dephosphorization agent

Farah Amalina, Santhana Krishnan, A.W. Zularisam, Mohd Nasrullah. *Biochar and sustainable environmental development towards adsorptive removal of pollutants: Modern advancements and future insight*. Pages 715-728.

Globally, environmental pollutants, involving emerging contaminants, are a developing issue. The tremendous growth of industry and the continuous emission of untreated effluents are significant challenges that pollute the ecosystem. Efforts are being focused on finding eco-friendly, cost-effective strategies to remediate various pollutants. Feedstock consists of organic wastes comprising food waste, compost, animal dung, agricultural residues, and sludge. Traditional treatment methods (primary and secondary treatment processes) are ineffective at mitigating or removing pollutants. Therefore, an effective, inexpensive, environmentally friendly tertiary treatment technique is urgently required. Biochar (BC) has intriguing uses in ecological functioning, such as pollutant removal, carbon emissions mitigation, and wastewater treatment. Various types of adsorbents (BCs), such as pristine and engineered BC, are utilized for the separation or remediation of heavy metals (HMs), polychlorinated dibenzo-p-dioxins (PCDDs), dibenzofurans (PCDFs), polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs) and organochlorine pesticides from polluted areas to promote sustainable development. This paper provides critical insight into BC derived from various biomass feedstocks for the adsorptive removal of pollutants. This article also examines numerous research that offers alternatives for environmental conservation and management, as well as the modern advancements of BC for environmental protection. The potential of various agricultural waste products and their ability to absorb contaminants was discussed. The challenges and future insight of research on the surface-based removal of pollutants were also explored.

- **Keywords:** Biochar; Contaminants; Biochar hazard; Environmental sustainability; Future insight

Amirhosein Ghozatfar, Saeed Yaghoubi, Hamideh Bahrami. *A novel game-theoretic model for waste management with waste-to-energy and compost production under government intervention: A case study*. Pages 729-746.

Due to leachate contamination in groundwater and also soil, global concerns about improper waste management are today raising. On the other hand, with the emergence of the circular economy, increasing the recycling rate, reducing the landfilling rate, and producing by-products such as energy and compost from waste have become particularly important. In this regard in this paper, a chain consisting of a collector, a municipality, a compost plant, and a power plant is considered in a municipality-led Stackelberg game under government intervention. Indeed, the government supports citizens, the compost plant, and the power plant with subsidies to control the prices economically and sets penalties for greenhouse gas (GHG) emissions and leachate infiltration. The collector collects waste through two competitive channels: one from the city's trash bins and the other through buying recyclable waste from citizens, whereas each channel has its collection function. The municipality makes environmental efforts such as increasing people's awareness and investing in technology level to separate and treat leachate. The municipality also receives a fee from the collector for allowing the collection of recyclable waste. On the other hand, the compost and power plants produce compost and energy from waste and price their product based on the level of environmental efforts such as leachate treatment and GHG control, respectively. A real example has been finally implemented for the Tehran Waste Management Organization and the sensitivity analysis is presented. The results have shown that the source separation rate 72.36% and the recycling rate 69.62% of the ordinary waste channel are the highest and the landfilling rate 4.09% is the lowest in the best government policy, which is environmental efforts compared to other policies; Moreover, the profit of the members is the maximum in this policy.

- **Keywords:** Waste management; Game theory; Circular economy; Energy; Government intervention; Technology level

Everton Gripa, Sarah Dario Alves Daflon, Ronei de Almeida, Fabiana Valéria da Fonseca, Juacyara Carbonelli Campos. *Landfill leachate treatment by high-pressure membranes and advanced oxidation techniques with a focus on ecotoxicity and by-products management: A review*. Pages 747-764.

Landfill leachate that primary and/or secondary technologies have treated needs to be subjected to further purification to meet local discharge limits due to its heavy macro and micro-contaminant load. In this sense, advanced oxidation process (AOP) and membrane-based technologies (i.e., nanofiltration [NF] and reverse osmosis [RO]) are commonly employed as polishing steps to meet legislation requirements. However, membrane-based techniques do not destroy pollutants but produce concentrated streams that must be managed. AOPs can generate sludge and by-products of higher toxicity than their precursors in raw leachate. In this context, this study reviews the ecotoxicological risks and pollution impacts of landfill leachate (1), identifies the weakness of the current leachate ecotoxicological studies to provide recommendations for future investigations (2), outlines the relevance of membrane-based and advanced oxidation techniques to manage landfill leachate (3), and proposes integrated treatment options for landfill leachate purification (4). Different combined methods to ensure proper wastewater purification characterize the leachate treatment chain. Biological processes followed by RO have showcased a significant trend within the leachate treatment chain. These systems operate with macro and micro-pollutants removal higher than 90%. On the other hand, managing treatment's by-products is challenging. An ozone-based technique could be integrated downstream to promote membrane concentrate and sludge mineralization. Combining membrane and ozone-based processes is promising to overcome concentrate management and toxicity issues. However, high-energy demand might render this kind of treatment configuration unfeasible, especially in small and middle-size landfills from remote sites. In this sense, landfill gas utilization and developing support energy systems based on renewables are critical in closing the leachate treatment loop.

- **Keywords:** Advanced oxidation process; Contaminants of emerging concern ecotoxicity; Landfill leachate; Nanofiltration; Reverse osmosis

Shuqiong Luo, Yali Ge, Minghui Zhao, Lei Yang, Jun Ren. *Application of microwave hydrothermal synthesis for the solidification of copper: Effect of heavy metal content and microwave time*. Pages 765-774.

The synthesis type and heavy metal content significantly affect the performance of microwave hydrothermal synthesis. This synthesis approach has lower energy consumption and shorter reaction time for consolidating the heavy metals in the tobermorite lattice. The goal of this study was to investigate the influence of microwave reaction time and copper (Cu) content on the preparation of Cu-substituted tobermorite (Cu-tobermorite). Fumed silica, calcium hydroxide and copper chloride dihydrate were used to prepare the Cu-tobermorite under a liquid-solid ratio of 30 mL/g, reaction temperature of 220 ℃, and (Ca+Cu)/Si ratio of 0.83. The effect of reaction time (2 h and 4 h) and Cu content (Cu/Ca ratios are 0, 0.05, 0.1, 0.15 and 0.2) on the microstructure and morphology of the Cu-tobermorite were investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM) and thermogravimetry (TG), and Fourier-transform infrared (FTIR) spectroscopy. Moreover, the solidification efficiency was assessed by inductively coupled plasma-optical emission spectrometry (ICP-OES). The results showed that the main products of microwave synthesis were Cu-tobermorite and tobermorite, while the conventional hydrothermal synthesis products were Cu-tobermorite and gyrolite. Prolonging the elongation of the reaction time did not change the type of hydration product. Both microwave and traditional hydrothermal synthesis of tobermorite solidified Cu with a solidification rate of almost 100%. However, the microwave method

provided a 1/7th shorter reaction time and less than 10% of the energy composition (< 10%

- **Keywords:** Microwave hydrothermal synthesis; Copper content; Tobermorite; Energy consumption; Leaching

Xinming Qian, Zhengrun Huang, Juncheng Jiang, Xingyu Shen, Mingzhi Li, Mengqi Yuan, Qianran Hu. *Physical evidence and system theory based accident investigation of strongly constrained environments: A case study*. Pages 775-785.

Flammable gas leaked from pipelines is easy to cause explosion accident. The consequences of accident are amplified in strongly constrained environments near the pipelines. In this paper, a gas leakage and explosion accident in Beijing is analyzed using field investigation and relevant experimental analysis techniques, and the complete investigation process of accident cause based on physical evidence is displayed. Some theoretical analysis models are introduced to explore the causes of this type of accident from a system perspective. The laws of explosion damage of building structures in strongly constrained environments are also summarized. The results indicate that the gas leaked from the end of the hose was excited by an electric spark in the electrical box causing this explosion and a gas explosion with a TNT equivalent of 2.73–4.28 kg is sufficient to damage a large number of walls of civilian buildings. The pressure difference between the two sides of structures and the duration are decisive factors in the degree of damage. Cause analysis shows that human error needs to be avoided through education and supervision. The study can provide theoretical references for the investigation of explosion accidents, as well as improvement of energy management system.

- **Keywords:** Accident investigation; Gas explosion; Cause analysis; STAMP; Structure response

Shihang Li, Hui Cheng, Shuda Hu, Guoxiang Wen, Ankang Zhou, Changgeng Gui, Liang Yuan, Fubao Zhou. *Study on the influence of built-in open-hole dust cleaner on the cleaning performance of cartridge filter*. Pages 786-799.

Pleated cartridge dust collectors are widely used in various industrial production environments, in its use, pulse-jet cleaning is a crucial step. Despite the importance of pulse-jet cleaning, there was a widespread problem of uneven cleaning in the upper part of the filter cartridge. In this paper, a built-in open-hole dust cleaner (BODC) was developed to improve the pulse-jet cleaning performance, ameliorate the problem of uneven cleaning and prolong the filter cartridge's service life. The filtration and pulse-jet cleaning test system was established to verify the effect of BODC. Based on the comprehensive comparison and analysis of pulse-jet pressure at the four types of measuring points, the best BODC in this experiment is 6 mm 4 holes with composite pressure of 1.52 MPa. The best BODC and ordinary nozzle were compared with respect to pressure drop. The results showed that the change rule of pressure drop of BODC is similar to that of the ordinary nozzle. The average filtration cycle of BODC and ordinary nozzle was 1300 s and 928 s, respectively. The dust emission concentration of the dust collectors of both cleaning methods during filtration was 1.354 mg/m3 and 1.412 mg/m3, respectively. A significant improvement in cleaning uniformity has been demonstrated when the BODC is used. Ultimately, the best BODC in this experiment was applied on site at the excavation face of Donghuantuo Coal Mine, which resulted in an average dust removal efficiency of 95.2% for total dust and 93.2% for respirable dust, with no residual dust left in the upper part of the filter cartridge after cleaning.

- **Keywords:** Filter cartridge; Pulse-jet; Cleaning uniformity; Peak positive pressure; Cleaning cycle; Dust concentration

Qing-Yun Zhou, Bei Li, Yi Lu, Jie Chen, Chi-Min Shu, Ming-shu Bi. *Dynamic risk analysis of oil depot storage tank failure using a fuzzy Bayesian network model*. Pages 800-811.

This paper presented a fuzzy Bayesian network (FBN) model for failure risk analysis of oil storage tank leakage. The Bow-tie model for storage tank failure in oil depots was established and used to determine key risk factors. Fuzzy set theory and expert judgments were used to calculate the prior probability of basic events, after which the model was mapped to a Bayesian network. The probability of storage tank failure was calculated as 7.80 E-02. As new evidence was obtained, probability updating was tested using forward inference. Posterior probability of a basic event, seal gasket aging, showed the greatest risk increase, from 1.05 E-02–1.10 E-01. Using these newly acquired key factors, probability adaptation was used to conduct a dynamic analysis of storage tank failures and the consequence states. The dynamic failure probability was found to increase by 28.67 %. The model underwent sensitivity analysis and literature data analysis. This fuzzy Bayesian network model is beneficial to dynamic risk analysis in oil depot management. The findings can be used to reduce the likelihood of oil tank failure and decrease the severity of accidents. Suggestions were made, for site engineers and management, to reduce the risk of hazardous events.

- **Keywords:** Bow-tie model; Leakage failure; Fuzzy set theory; Dynamic failure probability; Sensitivity analysis

Chaowei Wang, Chang'an Wang, Maoyun Luo, Liangxu Dai, Pengqian Wang, Defu Che. *Simulation study on fuel-nitrogen migration characteristics of oxy-fuel co-combustion of various ultra-low volatile coal-based solid fuels*. Pages 812-822.

The co-combustion of various ultra-low volatile coal-based solid fuels (UVCFs) under oxy-fuel condition could consume semi-coke and residual carbon cleanly and efficiently. However, the fuel-nitrogen (fuel-N) migration behaviors of various UVCFs blends in O2/CO2 atmosphere are still unclear. In addition, the heterogeneous reactions on surfaces of char could also affect the synergistic effects between various UVCFs blend. Here, the fuel-N migration features of various UVCFs in O2/CO2 atmosphere were investigated by Chemkin simulation and the oxy-fuel co-combustion mechanism of various coal-based solid fuels (OCF mechanism) included heterogeneous reactions was developed. Moreover, the methods of sensitivity and rate of production analyses were both employed to clarify the synergistic effects on nitrogen conversion pathways of various blends. The heterogeneous reaction between char and NO (R15) is the key reaction for NO reduction in primary zone. The free radicals OH and H provided by UVCFs could react with main NO precursors NCO, HNCO, HOCN, NH and NH2 to generate NO. The conversion pathways of HCN to NO are more complex than those of NH3 to NO. The rises of residual carbons proportions and temperature in primary zone (T1) could both reduce the NO formation amount due to the promoted R15. The sensitivity coefficients (S) on NO formation of 50% SS/50% CR blend in the burnout zone are lower than those of 50% SS/50% FR blend. The transformations of HNCO, HNO and NO2 to NO and the heterogeneous reactions of NO could both be enhanced with the O2 concentration in burnout zone. The increasing burnout air position (Pb) results in the rise of NO generation owing to that the NO reducing reactions R15 and R16 are greatly inhibited with the Pb raised. The present study could be beneficial for the clean and effective utilization of UVCFs, together with the reduce of NOx emission and realization of carbon neutral in China.

- **Keywords:** Carbon neutral; Oxy-fuel co-combustion; Fuel-nitrogen migration; NOx formation; NOx reduction Mechanism

Sonu Saini, Ramesh Chander Kuhad, Krishna Kant Sharma. *Valorization of rice straw biomass for co-production of bioethanol, biopesticide and biofertilizer following an eco-friendly biorefinery process*. Pages 823-836.

Combustion and depletion of fossil fuels, open burning of agricultural wastes, and use of hazardous chemicals in biofuels production route are some major challenges among scientific community. In the present study these obstacles were mitigated simultaneously. Initially, rice straw biomass was delignified using a combined eco-friendly laccase-assisted sodium chlorite (LASC) pretreatment. The combined pretreatment strategy of rice straw biomass reduced 55.6% lignin and increased the total available carbohydrate by 1.43 fold. Further, enzymatic digestion of LASC pretreated rice straw using a formulated cellulase cocktail from Aspergillus flavus MDU-5 and Trichoderma citrinoviride MDU-1 liberated 526.68 mg/g sugars with high saccharification yield (84.0%). The enzymatic hydrolysates thus obtained were found to contain 7.43–16.78 g/L sugars. The cellulolytic hydrolysates when fermented with Saccharomyces cerevisiae NCIM-3640 produced 3.02–7.28 g/L bioethanol, with high yield (72.96–85.31% of the theoretical value). Parallelly, lignin extracted from waste pretreatment stream showed biopesticidal activity against the larvae of H. armigera; whereas, the evaluation of residual material (after hydrolysis and fermentation) exhibited biofertilizer properties. These findings suggests that the environmentally benign LASC pretreatment, cellulase cocktail, and utilization of waste stream for the production of biopesticide and biofertilizer may provide a promising strategy in the development of holistic lignocellulosic biorefinery process.

- **Keywords:** Rice straw; Biorefinery; Pretreatment; Bioethanol; Biopesticide; Biofertilizer

Xiaochen Cheng, Chenyang Duan, Pei Yang, Yongrui Pi, Hailiang Qi, Zhengkang Sun, Shihua Chen. *Effective adsorption of crystal violet onto magnetic nanoparticles decorated bacteria: Kinetic and site energy distribution analysis*. Pages 837-846.

The discharge of crystal violet wastewater will cause extremely serious harm to the natural environment and human health, due to its certain toxicity and carcinogenicity. The adsorption characteristics and mechanism of crystal violet on magnetic nanoparticles decorated bacteria (Fe3O4 @bacteria) were investigated especially the adsorption kinetic, equilibrium, mass transfer mechanism, and site energy distribution analysis. With the initial concentration of crystal violet 40 mg/L, pH= 4, the addition of 0.003 g Fe3O4 @bacteria, after adsorption for 2 h under 25 °C, the static maximum adsorption capacity of crystal violet was up to 114.8 mg/g, which was 2.07 times that of Fe3O4 under the same conditions. Fe3O4 @bacteria could be recycled more than 6 times, also exhibited a 76.2% reduction in COD for actual dyeing wastewater. The adsorption data fitted well with the Temkin isotherm model, Elovich kinetic, and pseudo-second-order kinetic models. As for the mass transfer mechanism of the adsorption process, the IPD model was more suitable to describe the mass transfer process of the crystal violet adsorption by Fe3O4 @bacteria, while the intraparticle diffusion is not the only mechanism controlling the adsorption process. The adsorption process is spontaneous and exothermic according to the thermodynamics study. Based on the analysis of site energy distribution, the biosorbent had a heterogeneous surface and most of the crystal violet sorption occurred on the sites with energy over 13.0 kJ/mol, which supported that crystal violet sorption was physical-chemical sorption. Therefore, the magnetic nanoparticles

decorated bacteria can serve as promising adsorbents to eliminate the organic dye pollutants caused by textile industry.

- **Keywords:** Fe3O4@bacteria; Crystal violet; Adsorption characterization; Site energy distribution; The adsorption mechanism

Fenghui Wu, Minjie He, Guangfei Qu, Ting Zhang, Xinxin Liu. *Synergistic densification treatment technology of phosphogypsum and aluminum ash*. Pages 847-858.

Phosphogypsum and aluminum ash are typical bulk industrial solid wastes produced by phosphorus chemical and aluminum electrolysis industries respectively, both of which are characterized by large yield, low utilization rate and high environmental risk. In this article, high-density blocks were synthesized for the first time by densification treatment with phosphogypsum and aluminum ash. The mechanical and waterproof properties of the blocks formed after densification treatment under different ratios, densification pressures and curing time were also investigated. The experimental results indicate that the blocks treated by densification demonstrate a remarkable comprehensive performance under the optimal conditions of a ratio between phosphogypsum and aluminum ash of 1:9, densification pressure of 300 MPa and curing time of 5 d. Under such conditions, the compressive and flexural strength of the blocks are 58 MPa and 1.7 MPa respectively, with water absorption rate of about 5.3% and softening coefficient of 0.99. The leachable efficiency of toxic and harmful elements in the block materials is low, meeting the requirements for environmental protection, and thus densification treatment can be used for the harmless treatment of solid waste. The method provides a feasible research idea for simulating the change of underground minerals under the action of surface pressure and exploring the harmless and resourceful treatment of bulk solid waste. The technology is expected to be applied in the field of high-density filling and building materials prepared from solid waste.

- **Keywords:** Phosphogypsum; Densification; Aluminum ash; Non hazardous treatment

Maghsoud Abdollahi Haghghi, Amirhossein Hasanzadeh, Ebrahim Nadimi, Antonio Rosato, Hassan Athari. *An intelligent thermodynamic/economic approach based on artificial neural network combined with MOGWO algorithm to study a novel polygeneration scheme using a modified dual-flash geothermal cycle*. Pages 859-880.

Flash-based geothermal cycles correspond to environmentally friendly and cost-effective processes in a renewable framework and provide an opportunity for combined cycles. However, these cycles are characterized by significant energy losses and their waste stream's low/medium operational temperature is the principal defect for managing multiple generation arrangements without assisting other energy resources. Hence, the main aim of this study is to propose a novel polygeneration scheme, integrated with a dual-flash geothermal cycle equipped with self-superheaters, able to mitigate the discussed defect. A new coupled series and parallel design of energy recovery is established, allowing to increase the compatibility of combined cycles and enable a larger production. This design encompasses a single-effect refrigeration cycle, a modified transcritical CO2 cycle, a polymer electrolyte membrane electrolyzer, and a thermal desalination cycle. The proposed process is examined from thermodynamic, sustainability, and economic (exergoeconomic and net present value analyses) points of view. Besides, a detailed sensitivity study is conducted by which the trend of performance variables in response to the increasing five main decision parameters is viewed. Afterward, an intelligent approach relying on an artificial neural network is built to learn and validate the behavior of defined objective functions (exergetic efficiency and

products' levelized cost). Moreover, a multi-objective grey wolf optimization (MOGWO) procedure endeavors to optimize the operation of the system. According to the results of this study, flash tank 2's inlet pressure is the effective parameter, and its mean sensitivity index equals 0.289. Besides, the aforementioned objectives are gauged at 37.45% and 0.0625 $/kWh, respectively.

- **Keywords:** Multi-stage waste management; Dual-flash geothermal cycle; Transcritical CO2 cycle; Polygeneration; Multi-objective grey wolf optimization; Artificial neural network

Yayong Yang, Feng Chen, Tianchi Shen, Agamuthu Pariatamby, Xiaoqiang Wen, Mi Yan, Ekkachai Kanchanatip. *Catalytic depolymerization of waste polyethylene terephthalate plastic in supercritical ethanol by ZnO/γ-Al2O3 catalyst.* Pages 881-892.

In order to minimize the environmental impact from polyethylene terephthalate (PET) plastic waste, catalytic depolymerization was employed to break down PET into useful diethyl terephthalate (DET) monomers. This research investigated the depolymerization of waste PET in supercritical ethanol (SCE) catalyzed by ZnO/γ-Al2O3 catalysts. The effect of the types of γ-Al2O3 (neutral and acidic) support, ZnO loading and catalyst dosage were studied. The catalytic efficiency of the catalysts was evaluated by the yield of DET obtained from the catalytic depolymerization of waste PET in SCE at 270 °C and 60 min reaction time. The results revealed that the highest DET yield of 92.2% could be obtained with 7.5 wt% ZnO supported on acidic γ-Al2O3 with catalyst dosage of 5% by weight of waste PET. NMR analysis indicated that the catalytic depolymerization process was complete since there were no PET polymer residues in the liquid. In addition, the ZnO/γ-Al2O3 catalyst also had good stability after five cycles of reuse, its catalytic activity was still satisfactory. The findings suggested that catalytic depolymerization in SCE is a promising alternative for converting waste PET into valuable materials.

- **Keywords:** Waste PET; Diethyl terephthalate; Supercritical ethanol; ZnO/γ-Al2O3; Recycling

Sally R. Osman, Bishoy E. Sedhom, Sahar S. Kaddah. *Optimal resilient microgrids formation based on darts game theory approach and emergency demand response program for cyber-physical distribution networks considering natural disasters*. Pages 893-921.

In this paper, novel multi-objective microgrids (MGs) formation method-based darts game theory optimization algorithm is proposed. The main objectives are to minimize the total losses, amount of load-shedding, and total restoration cost while ensuring a variety of topological and electrical constraints. The network graph theory represents the formed MG, and the non-linear equations of power flow and loss calculations are adopted in the MG formation model. In the proposed model, the DRERs include diesel generators, fuel cells, micro-turbines, and renewables wind and PV units with energy storage systems. The demand response program includes curtailable loads to improve load profile reduction during peaks. To assess the system's resiliency under extremely inevitable incidents, resiliency metrics are applied. To validate the effectiveness of the proposed approach, the modified IEEE 33-bus test system is utilized. Single-fault and multiple faults disaster case studies are performed with and without considering the emergency demand response program (EDRP). The results show the effect of EDRP in minimizing system losses, load-shedding, restoration cost, and improving the resiliency metrics after natural disasters. Finally, the analytic hierarchy process (AHP) model indicates the most efficient operation scenario while achieving the system objectives considering the problem alternatives.

- **Keywords:** Cyber-physical distribution network; Microgrid; Distributed renewable energy resources; Darts game theory; Demand response; Resilience metrics

Xingwei Zhen, Yinan Ning, Wenjie Du, Yi Huang, Jan Erik Vinnem. *An interpretable and augmented machine-learning approach for causation analysis of major accident risk indicators in the offshore petroleum industry*. Pages 922-933.

The offshore petroleum industry faces continuous stress and threats of major accidents. A complete and well-designed spectrum of indicators could help identify and improve the understanding of the status of all relevant hazards for managing various risks on offshore installations. The Petroleum Safety Authority (PSA) in Norway develops a project of extended indicators, i.e., "Trends in risk level" (RNNP), which uses an assortment of risk indicators to reflect the status and trend of the risk level. However, a simple statistical approach is insufficient to see into the causes behind the risk indicators. This paper proposes an interpretable and augmented machine-learning approach for causation analysis of major accident indicators. The proposed methodology integrates the K-means SMOTE technique for data augmentation to promote the performance of machine-learning algorithms. Armed with the analytical approach, the problem of lack of sample data is solved and the importance of the features of risk indicators is analyzed. Furthermore, a case study is presented to augment and analyze the two types of risk indicators associated with major accidents recorded from 2005 to 2021. The effectiveness of the proposed approach is demonstrated by the case study. It can provide an effective tool to help find out which type of features deserves more attention in risk management and target risk reduction measures that could be taken to strengthen safety on offshore installations.

- **Keywords:** Risk indicators; Machine learning; SHAP; K-means SMOTE; DFU; Barrier

Boo-Hyoung Bang, Chanwoo Park, Sam S. Yoon, Alexander L. Yarin. *Numerical modeling for turbulent diffusion torch of flammable gas leak from damaged pipeline into atmosphere*. Pages 934-945.

Assessment of pipeline safety is of paramount significance for safety of petrochemical plants. Any leakage of flammable gas from a pipeline poses a potential risk of an explosion followed by fire. Following a leak, a non-burning inert gaseous jet is first formed and, thereafter, ignition happens and an exothermal torch or flame occur. Safety assessments of such a scenario can be made by considering free-boundary-layer turbulent flows of fuel propagating in the surrounding atmosphere based on Prandtl's mixing length theory. That implies modeling the fields of fuel/oxidizer concentrations, velocity, and temperature, and the overall shape of the axisymmetric inert jets and exothermal diffusion torches. Axisymmetric turbulent boundary layer equations have been solved numerically, and these solutions have been compared with self-similar solutions for inert jets. The comparison confirms that the difference between the numerical and self-similar solutions in the longitudinal velocity profile is within 1%. Furthermore, the numerical model predicts the fuel concentration within an uncertainty level of 15% when compared with the experimental data. In an exothermal torch, the combustion temperature keeps increasing until the fuel is depleted. Outside the fuel zone, the temperature of the torch cools abruptly in the radial direction. The longitudinal velocity of an exothermal torch is moderately higher than that of an inert jet because of the thermal expansion. In this work, results of parametric studies are presented for various values of the Reynolds number, which can be useful for petrochemical engineers who assess the risk level associated with potential fire hazards caused by pipeline leakages.

- **Keywords:** Turbulent combustion torch; Pipeline leakage; Diffusion flame; Fire hazard; Self-similar solution; Prandtl's mixing length theory

El Farouk Omar Merouani, Milad Ferdowsi, El-Hadi Benyoussef, Luc Malhautier, Gerardo Buelna, J. Peter Jones, Michèle Heitz. *Biological mitigation of methane in presence of xylene and ethylbenzene in biofilters: Effect of pollutants concentrations and empty bed residence time*. Pages 946-960.

Landfill gas emissions cause serious environmental concerns due to the presence of methane (CH4), an important greenhouse gas (GHG) and several harmful volatile organic compounds (VOCs) such as xylene (X) and ethylbenzene (EB). A series of 9 up-flow biofilters (3 sections of 0.3 m each) packed with inorganic materials were used to eliminate CH4 as a single pollutant, a binary mixture of X and EB and a ternary mixture of CH4, X and EB. The CH4 concentration range was 2000–10000 ppmv while the VOCs (X and EB) individual concentrations were 200, 400 and 600 ppmv for empty bed residence times (EBRTs) ranging from 2.25 to 9 min over a period of 242 days. The highest CH4 removal efficiency (RE) in the ternary mixture was 41 ± 3% at a CH4 concentration of 2000 ppmv and X and EB individual concentrations of 200 ppmv for an EBRT of 9 min. Meanwhile, the highest X and EB-REs of 58 ± 3 and 57 ± 3% were obtained respectively, at the same concentrations of the components but at a shorter EBRT of 4.5 min. Almost 40% of CH4 biodegradation took place on the top section of the bioreactor while 50–60% of the VOCs biodegradation occurred in the middle section.

- **Keywords:** Bioprocess; Biofiltration; Biodegradation; Greenhouse gas; VOC; Inhibition

Ruyuan Jiao, Jinbo Zhang, Xiaofang Yang, Xinmeng Zhu, Wei Gao, Dongsheng Wang. *Key odorant identification and odor treatment technology evaluation during the chemical synthesis process of typical pesticide*. Pages 961-969.

Odor pollution has become one of the important environmental problems in China. In this study, Gas Chromatography Ion Mobility Spectrometry (GC-IMS), Gas Chromatography Mass Spectrometer (GC-MS) and Flame Ionization Detector (FID) were combined to obtain comprehensive information of the odor produced during the production of Captan, a common pesticide, and to evaluate the efficiency of the odorant treatment techniques utilized by the manufacturer studied. Based on our findings, refining, an important phase during the production process of Captan, was found to be the most important factor in determining the type and the concentration of the odorant produced. Of the odorants found during the production process, perchloromethylmercaptan (CCl3SCl) and other chlorine-containing compounds are the key odorants during the production process based on the calculation of odor activity value (OAV). The current odorant treatment utilized by the manufacturer studied showed about 40 % removal rate. However, the odorant treatment produced a new odorant, dimethyl disulfide. Therefore, a much more targeted odorant treatment technique without the production of new odorants is desired and should be utilized.

- **Keywords:** Chromatography Ion Mobility Spectrometry (GC-IMS); Gas Chromatography Mass Spectrometer (GC-MS); Characteristic volatiles fingerprints; Key odorant; Captan