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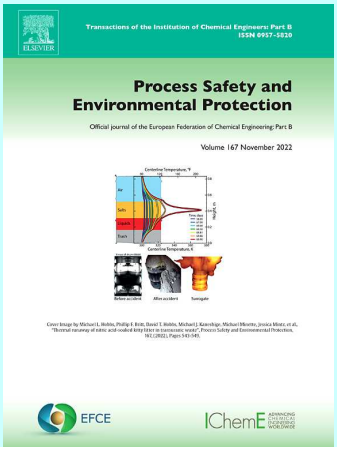

Shuangli He, Jinghang Ren, Peng Cao. *Green Ce-based honeycomb catalyst with excellent water and sulfur dioxide resistances for low-temperature selective catalytic reduction of NOx with ammonia*. Pages 1-16.

Low-temperature selective catalytic reduction (SCR) is effective and promising for converting NOx in flue gas into N2, with wide application prospects. However, low-temperature denitration (DeNOx) catalysts are susceptible to SO2 and H2O poisoning. Here, we prepared a monolithic Mn-Fe-Ce/Al2O3 catalyst that exhibited excellent DeNOx performances at low temperatures. At 110 °C, the NO conversion rate of the catalyst was> 90%, exhibiting excellent resistances to H2O and SO2·H2O and SO2 are introduced at the same time, the efficiency is as high as 73%. Furthermore, The catalyst has a porous structure with abundant chemisorbed oxygen spices and exposed active, the reaction pathway on the catalyst proved to be the L-H mechanism based on in situ DRIFTS. This study also explored the mechanisms of low-temperature SCR catalyst poisoning by SO2 and H2O, providing insights into the effects of SO2 and H2O and theoretical support for the development of poisoning-resistant low-temperature SCR catalysts.

- **Keywords:** Low-temperature SCR; H2O and SO2 resistance; Ce-based catalyst; Influence mechanism

Priyanka Prabhakar, Raj Kumar Sen, Venkatesh Mayandi, Monika Patel, B. Swathi, Jeet Vishwakarma, V.S. Gowri, Rajamani Lakshminarayanan, D.P. Mondal, Avanish Kumar Srivastava, Neeraj Dwivedi, Chetna Dhand. *Mussel-inspired chemistry to design biodegradable food packaging films with antimicrobial properties*. Pages 17-29.

Environmental pollution owing to plastic waste is a growing global issue. Packaging materials generate the maximum plastic waste, weighing 141 million tonnes/year. Driven in part by pressure from progressively environmental-conscious consumers, many industries are shifting their means of packing food products to more sustainable options.

To promote sustainability, the present work investigates the potential of mussel-inspired polydopamine (pDA) chemistry to develop biodegradable antimicrobial food packaging materials. The food packaging films are designed using unique material combinations including polyvinyl alcohol (PVA), pDA, glycerol, and epsilon-polylysine (εPL). Along with exceptional biodegradability (46% in 1 week), these films demonstrate superb antibacterial activity against both gram-positive and gram-negative bacteria, as well as good thermal and mechanical properties. Additionally, these packaging films display excellent UV shielding properties that can protect the food from UV-induced photodegradation. Overall, this study uncovers numerous novel phenomena of mussel-inspired polydopamine chemistry to address major issues with plastic-based food packaging, such as biodegradability, microbial contamination of food, light-induced food spoilage, and so on.

- **Keywords:** Mussel-Inspired; Polydopamine; Epsilon-polylysine (εPL); Sustainable Food Packaging; Antimicrobial

Deepika Arya, Santanu Bandyopadhyay. *Stochastic Pinch Analysis to address multi-objective resources conservation problems with parametric uncertainties*. Pages 30-48.

An emphasis on sustainable growth helps decrease the initial capital and reduce the impact of industry on an ecologically sensitive environment through resource conservation. Pinch Analysis serves as a valuable tool to identify the potential for resource conservation, waste minimization, and resource costs. However, there are inherent uncertainties associated with these resource conservation networks. The concept of Pinch Analysis is broadened to multi-objective resource conservation problems incorporating parametric uncertainties in this paper. The objective functions are combined to form a single compound objective function using the weighted sum approach. For the compound objective function, prioritized sequences (or resource combinations) are generated through multi-objective prioritized costs to accommodate parametric uncertainties. The multi-objective prioritized cost vs. weights curve helps determine the unique prioritized sequences for different range of weights to achieve optimal solutions. An exact analytical expression for the maximum number of prioritized sequences is also derived. Furthermore, a method is presented to construct the complete Pareto-optimal front to represent all optimal solutions graphically. Two illustrative examples, the hydrogen conservation problem with two objectives (cost and emission) and the water conservation problem with three objectives (cost, land requirement, and emission), demonstrate the proposed method's utility and efficacy.

- **Keywords:** Multi-objective optimization; Parametric uncertainties; Resource conservation; Pinch analysis; Chance-constrained programming; Pareto-optimal front

Assem A. Dewidar, George A. Sorial, David Wendell. *Performance evaluation of fungal biotrickling filter for styrene destruction: Experimental and artificial neural networks modeling*. Pages 49-60.

Removal of styrene vapors was investigated using a fungi-cultured biotrickling filter (BTF) in the presence of rhamnolipid. Evaluations at empty bed residence times (EBRTs) of 90, 60, and 30 s and inlet loading rates (LRs) ranging from 25.5 to 186.1 g m−3 h−1 were conducted. The maximum elimination capacity (EC) of 173.7 g m−3 h−1 was obtained at an inlet LR of 186.1 g m−3 h−1 at 90 s EBRT. Reducing the EBRT to 60 and 30 s resulted in decline of removal efficiency (RE). The performance of BTF was modeled using artificial neural network (ANN) to predict styrene RE using measurable inputs, inlet LR, EBRT, and pressure drop. The model performance was assessed by mean square error and overall coefficient of correlation. The influence of different input parameters on the output was analyzed using casual index. Styrene removal was positively influenced by the increase in

EBRTs, negatively impacted by its inlet LRs, while pressure drop had a negligible effect. The BTF was then exposed to intermittent loading phases by varying operational conditions during the non-loading periods. The results from this study confirmed that rhamnolipids could enhance the BTF performance for handling transient load variations at unsteady-state conditions.

- **Keywords:** Biotrickling filter; Intermittent loading; Modeling; Neural networks; Rhamnolipids; Styrene

Shaik Afzal Mohiuddin, Ajay Kumar Kaviti, T. Srinivasa Rao, S.R. Atchuta. *Experimental assessment of productivity and sustainability of nanoporous Cr-Mn-Fe oxide nanocoating in solar-powered desalination*. Pages 61-71.

Solar-powered desalination is a cost-effective technology to produce drinkable, potable water using energy from the sun. However, its use in domestic and industrial applications is minimal because of its low daily production. This study produced a novel nanoporous Cr-Mn-Fe oxide nanocoating by modulable chemical oxidation at a temperature of around 90 ℃ in an acidic mixture of 21–34 wt% conc.H2SO4, 37.5–53 wt% distilled water & 15–30 wt% sodium dichromate salt on a mirror-polished SS202 sheet to act as a basin liner for the nanocoated solar still (NCSS). The optical characterization of nanostructure coating was done using Cary 5000 spectrophotometer and FTIR spectrophotometer for absorptivity (90%) and emissivity (14.4% at 300 ℃), respectively. It was found that the nanocoated solar still (NCSS) produced 36.36%, 28.62%, and 26.27% more distillate yield when compared with conventional solar still (CSS) for 1 cm, 2 cm, and 3 cm depth of water, respectively. Enviro-economic studies, energy matrices evaluation, and water quality analysis were performed to compute greenhouse gases emissions, carbon dioxide mitigation, carbon credit gained, energy-payback time (EPT), energy production factor (EPF), life cycle conversion efficiency (LCCE), and suitability of distilled water for drinking. The cost per liter (CPL) of desalinated water for NCSS was inferred to be 15.6% more economical than for a CSS and 81% more economical than packaged drinking water in India.

- **Keywords:** Nanocoating; Productivity; Enviro-economic; Energy matrices; Water quality; Desalination

Xiaodong Wang, Yongxun Dai, Chen Tian, Huize Zhang, Xiwen Li, Wenlong Liu, Weibing Li, Shaoping Kuang, Hongtao Tong. *Boosted photocatalytic removal of Cr(VI) using MoS2 modified g-C3N4/ZnFe2O4 magnetic heterojunction composites*. Pages 72-82.

Photocatalysts can be effectively recovered and reused by compounding with magnetic nanostructures. How to further improve the photocatalytic performance of magnetic heterojunction photocatalysts remains a great challenge. In this work, g-C3N4/ZnFe2O4 (CN/ZFO) magnetic heterojunction photocatalyst was first prepared and then modified with ultrathin MoS2 (CN/ZFO/MoS2) by simple ball-milling method. Then the photocatalytic removal of Cr(Ⅵ) performance of the prepared series photocatalysts was evaluated in detail. The optimum CN/ZFO/MoS2 can achieve 99.3% Cr(Ⅵ) removal under 200-min simulated sunlight illumination, which is much higher than CN/ZFO (54.0%). The enhanced photocatalytic performance benefits from the modification of MoS2, which improves the light absorption performance, facilitates the transfer of photogenerated carriers, increases the concentration of photogenerated carriers and promotes the effective separation of photogenerated carriers. This work provides a theoretical basis for further preparation of magnetic recyclable photocatalysts with high photocatalytic performance.

- **Keywords:** Magnetic photocatalyst; Heterojunction photocatalysis; Photocatalytic Cr(Ⅵ) removal; G-C3N4/ZnFe2O4/MoS2; Photocatalytic performance

V. Saravanan, S. Ashokkumar, N. Rajamohan, Sang-Woo Joo, Yasser Vasseghian, M. Rajasimman. *A mixed agro-waste based biofilter for the removal of methyl ethyl ketone: Kinetics and modeling*. Pages 83-96.

Biofiltration has grown worldwide, as an inexpensive and consistent air pollution control technology for the elimination of numerous organic compounds. In this work, the biofiltration of methyl ethyl ketone (MEK) has been studied. The agro-wastes namely pressmud and cornstack are mixed and used as packing materials for the removal of MEK. The performance of the biofilter has been explored over 200 days. Experiments are carried out in four periods. In every period, the biofiltration of pollutants is performed for various inlet concentrations (IC) of MEK (0.2–1.2 g m−3) and gas flow rates (GFR) (0.03 m3 h−1 to 0.12 m3 h−1). The biofilter performances are investigated by their removal rates, elimination capacity, temperature, pressure drop, carbon dioxide production, and variation of bed height at the time of operations. For the IC of 0.2 ± 10% g m−3 and GFR of 0.03 m3 h−1, the removal efficiency (RE) of MEK is 97% using the mixture of cornstack (80%) and pressmud (20%). The MEK removal efficiency decreases, when the cornstack ratio increases. The maximum RE is obtained at the IC of 1.2 g m−3 and GFR of 0.12 m3 h−1 for all the tested conditions. The pressure drop (PD) is also measured for all the operating conditions. It is found that the PD rises with an increase in height. The temperature is monitored throughout the biofiltration process. It is observed that an increase in RE leads to a rise in temperature in the biofilter. SEM images confirm the growth of microbes on the packing material. The kinetics of removal of MEK is investigated by using Ottengraf–van den Oever model.

- **Keywords:** Methyl ethyl ketone; Biofilter; Biofiltration; Kinetics; Agro wastes

R. Gharari, H. Kazeminejad, N. Mataji Kojouri, A. Hedayat. *Analysis of the gases distribution during a severe accident by coupling the MELCOR and FLUENT in WWER1000 containment*. Pages 97-111.

It is necessary to evaluate the released gases distribution (especially hydrogen) to avoid hydrogen accumulation and maintain containment integrity against the pressure loads due to its deflagration or detonation. For this purpose, this work uses coupling of the FLUENT and MELCOR to evaluate the produced gases distribution in the WWER1000/V446 during in-vessel and ex-vessel phases of the Station Black Out (SBO) along with Large Break Loss of Coolant Accident (LBLOCA). The results indicate that 30 cm mesh size is sufficiently fine to evaluate the gases behavior in the containment. Also, driving force of the hydrogen/carbon monoxide (CO) and steam are mainly in the form of the plume due to buoyancy effects and jet flow caused by momentum, respectively. Furthermore, hydrogen accumulates in the upper compartments more than in other areas and its average volume fraction reaches to 12.7% at the end of the calculations. In addition, it can be concluded that steam condensation on the walls increases the hydrogen volume fraction up to 2%.

- **Keywords:** Severe accident; Hydrogen distribution; MELCOR; FLUENT; WWER1000

Ahmad Bamasag, Fadl A. Essa, Z.M. Omara, Essam Bahgat, Abdulmohsen O. Alsaiari, Hani Abulkhair, Radi A. Alsulami, Ammar H. Elsheikh. *Machine learning-based prediction and augmentation of dish solar distiller performance using an innovative convex stepped absorber and phase change material with nanoadditives*. Pages 112-123.

As well known, the solar distiller is one of the introduced solutions to the freshwater shortage problem, but it is demerited by the low freshwater output. In this paper, a design modification that includes the use of a convex dish absorber instead of a flat absorber liner was proposed. Also, a circular stepped surface was used instead of the flat absorber surface. The modified solar distiller is nominated by dish solar distiller and abbreviated by DSD. In addition, a cotton wick was used as a wetting material for facilitating the evaporation process inside the distiller. Besides, the effect of different water heights in the steps was investigated for 0.50, 1, 1.50, 2, and 3 cm. Finally, the space under the dish absorber is filled with a phase change material (PCM) of paraffin wax mixed with CuO nanoparticles. Experimental results revealed that the best water depth over the steps absorber of DSD that provided the highest freshwater productivity was 1.50 cm, where the average daily yields of DSD (at 1.50 cm) and conventional distillers were reported as 6525 and 2800 mL/m².day, respectively. Then, the productivity of DSD was improved by around 133% over that of the conventional distiller. In addition, when using the phase change material, the average daily distillate of stepped DSD was improved by approximately 178% compared to that of the conventional solar still, where the distillate of conventional still and DSD with PCM at 1.50 cm water depth over the steps absorber of DSD was 2950 and 8200 mL/m².day, respectively. The water productivity of the three established solar distillers has been predicted using machine learning algorithms. Besides, the maximum thermal efficiency of DSD was obtained when using PCM at 1.5 cm water depth over the steps absorber of DSD, where it was 67.62% compared to 31.71% for the conventional distiller. The proposed machine learning algorithms succeeded in predicting water productivity with a high correlation coefficient of 0.99.

- **Keywords:** Solar distillation; Artificial intelligence; Wick, CuO nanoparticles; Stepped absorber

Hebatallah Mohamed Teamah, A. E. Kabeel, Mohamed Teamah. *Potential retrofits in office buildings located in harsh Northern climate for better energy efficiency, cost effectiveness, and environmental impact*. Pages 124-133.

The current study evaluates the potential measures for enhancing energy efficiency in a commercial building application. It is directed towards addressing Northern climate conditions that are scarce in literature. To highlight the recommended measures, a case study involving a two-storey office building that was built in the late 1970s in Ottawa, Canada is presented. As typical for commercial buildings in Northern climates, building heat is provided by natural gas. Cooling, lighting, and other building needs are supplied by electricity. The building current operational condition deviates from what is recommended by the building code. The authors were consulted to propose energy efficiency measures for the building. The building was simulated using the eQuest software. Verification of the simulation results was performed against historic site data. The model highlighted several parameters that can reduce energy consumption and greenhouse gas emission. Major influencers on energy consumption were: building envelope, water heating system, and building air tightness. Amongst them, increasing building air tightness is the cheapest to implement. On the other hand, the parameters that are functions of occupancy had minor effect on the reduction of energy consumption. A detailed economic analysis has been conducted to evaluate the feasibility of the proposed retrofit strategies. The analysis quantified that the wall, roof insulation, boiler

upgrade and building air tightness have a high impact on reducing energy consumption by more than 52%. The improvements have the potential to reduce the emissions by around 82 tons of CO2 per year. The return on investment was found to be 5 years. The incorporation of renewable energy to the building was also investigated. Solar energy is not commonly integrated in cold climates in most of the reported research. For the current study, a solar heating system was installed to supply needed hot water and a PV system is used for electricity generation. This causes the payback period to increase to 5.6 years if solar water heating is added and to 9.1 years with solar water heating and photovoltaic integration. Debt ratio and interest rate have detrimental effect on return on investment for the project. The results of the current study are valuable recommendations for people interested in retrofitting commercial applications in Northern climates.

- **Keywords:** Energy efficiency; Cost effectiveness; Environmental impact; Green energy

Alfred Oloo Ochieng, Tamer F. Megahed, Shinichi Ookawara, Hamdy Hassan. *Comprehensive review in waste heat recovery in different thermal energy-consuming processes using thermoelectric generators for electrical power generation*. Pages 134-154.

This paper presents a comprehensive review of recent studies in electrical power generation from various thermal-consuming processes. In particular, the paper concentrates on TEG technology in recovering waste heat from industrial applications such as chimneys and automotive engines. Studies conclude that TEGs have a lower conversion efficiency (ranging between 5% and 10%), leading to low power output. Also, they state that most of the available TEGs have low operating temperatures limiting their commercial use. Therefore, an effort is taken to understand the key parameters that influence the performance of a thermoelectric generator. It is shown that a large temperature difference across the module, high heat dissipation from the cold side of the TEG and using thermoelectric materials with a high figure of merit generally improve the performance of the thermoelectric generator system. TEG module's cold-side temperature has a large effect on the power output than the hot-side temperature. Several geometric optimization methods, such as flaps and heat spreaders under natural convection resulted in a 129% and 42% increase in TEG power output, respectively. The survey also shows that forced cooling using side-mounted fans produces 58.6% more power compared to the top-mounted fan on the heat sink. However, optimization in fan selection is required to ensure that the power produced by forced cooling is sufficient to run the fans and output higher than the natural convection cooling case. Several studies also show that most of the commercially available TEG modules made from Bismuth telluride suffer from low operating temperature (maximum of 2600 C) and have figure of merit of 1.2 maximum and low conversion efficiency (up to 5%). Recommendations are made to further research alternatives like SiGe alloys, clathrates, skutterudites, and complementary metal-oxide semiconductors with better temperature ranges and figures of merit.

- **Keywords:** Thermoelectric generator; Waste heat recovery; Automobiles; Industrial application; Working principle

Ying Zhang, Wei Mao, Ruohan Li, Yang Liu, Peng Wang, Zelin Zheng, Yuntao Guan. *Distribution characteristics, risk assessment, and quantitative source apportionment of typical contaminants (HMs, N, P, and TOC) in river sediment under rapid urbanization: A study case of Shenzhen river, Pearl River Delta, China*. Pages 155-168.

Shenzhen River (SZR) is a boundary river of two super-large modern cities and has important wetland ecological functions in the estuary, while it suffered unprecedented pollution during the past decades due to the rapid urbanizing of the catchment area. Twelve parameters of heavy metals (HMs), nutrients (N, P, TOC), and physicochemical indexes (pH, EC) of the SZR sediment from 8 typical sites were analyzed to explore their distribution, risk, and sources. The distribution of sediment parameters was closely related to the urban functional structure, basin topography, and anthropogenic control. Heavy metals (HMs) of SZR sediment were in a contamination degree order of Cd> >Cu> Zn> Pb> Ni> Cr, a combined risk of HMs and tremendous organic threat concentrated at the upper and middle reaches in the lower layer. HMs and nutrients in SZR sediments showed strong inner correlations but were limited influenced by physicochemical properties. Factor, clustering, and multiple linear regression analysis were comprehensively applied for the quantitative source apportionment. Industry-related sources and domestic wastewater were the major contamination sources, while the non-point sources like urban surface runoff, natural sources, and solid waste carrying should be paid special attention to considering their maintained increasing risk.

- **Keywords:** River sediment; Combined pollution; Risk assessment; Urbanization impact; Source apportionment

Marco Manetti, Maria Concetta Tomei. *Extractive polymeric membrane bioreactors for industrial wastewater treatment: Theory and practice*. Pages 169-186.

Treatment of industrial wastewaters with current technologies can be very challenging, due to the presence of toxic and persistent compounds and to unfavorable pH conditions, which exert toxic/inhibitory effects on the biomass. Extractive membrane bioreactor (EMB) is a promising technology capable to overcome these difficulties. The system ensures separation between "hostile" wastewater and the biomass, allowing the gradual release of contaminants in the bioreactor under a concentration gradient, through an absorptive/diffusive membrane. Depending on thermodynamic affinity, the membrane is permeable only to target compounds, thus ensuring a "selective" extraction. In this review, earlier PDMS and newest polymeric membrane reactors have been analyzed, highlighting their potentialities and the still open research issues. The effects of biofilm formation, reactor configuration and operative parameters, such as Hydraulic Retention Time and geometric configuration, have been discussed. Despite good results in terms of contaminants removal, these parameters strongly affect reactor performance and further investigations are necessary. Furthermore, data analysis showed that this technology is ready for upscaling and this step is crucial for a full evaluation of the feasibility of a technology that could bring a remarkable improvement for industrial wastewater treatment.

- **Keywords:** Extractive membrane bioreactor; Recalcitrant contaminant; Diffusive membrane; Industrial wastewater; Biomass inhibition; Biofilm control

Ahmad Al-Douri, Syeda Zohra Halim, Noor Quddus, Vasiliki Kazantzi, Mahmoud M. El-Halwagi. *A stochastic approach to evaluating the economic impact of disruptions in feedstock pipelines on downstream production*. Pages 187-199.

Reliability of feedstock supply is an important consideration for enhancing the safety and continuous operation of chemical plants. A critical component of the chemical and refining sectors is the extensive pipeline network which transports natural gas and hydrocarbon liquids from producing areas to refineries and chemical plants. Incidents involving spills or releases and shutdowns of those pipeline can occur due to a number of causes including corrosion, equipment malfunction, and excavation damage. These incidents involve economic, environmental, and safety consequences such as the cost of asset damage, lost commodities, cleanup requirement, and operational disruption. In this work, an appropriately developed stochastic framework is presented to determine the disruption impact of pipeline incidents on downstream chemical production. Incident data are statistically analyzed to determine meaningful distributions for incident rates, spill/release quantities, and pipeline shutdown durations. A case study on the production of propylene via three different pathways (crude oil, propane, and natural gas) is presented to illustrate the methodology and underline the variability of the process production impact due to variations in risk occurrence characteristics. Using specific process chemistry and mass balances, more precise risk profiles for the product shortfall and cost of lost sales can be generated.

- **Keywords:** Hazardous Materials Pipelines Safety; Economic Risk; Risk assessment; Uncertainty; Quantification

Chao Wang, Bingbing Feng, Peifang Wang, Wenzhou Guo, Xianjin Li, Han Gao, Bo Zhang, Juan Chen. *Revealing factors influencing spatial variation in the quantity and quality of rural domestic sewage discharge across China.* Pages 200-210.

Understanding the characteristics of domestic sewage discharge in different rural areas is an important prerequisite for effective sewage treatment. Here, we revealed the spatial variation in the water quantity and quality of rural domestic sewage and its influencing factors in 31 provinces and cities of China, based on a multi-factorial analysis. The results showed that the water quantity of rural domestic sewage discharge generally increased from Northwest to Southeast in China and the water quality had opposite pattern. The water quantity was positively correlated with water resources, gross domestic product, rainfall, and temperature, but negatively correlated with altitude. Water resources, with an influence weight of 25.04% by principal component analysis, had the greatest impact on the spatial variation in water quantity. Differently, gross domestic product, which was directly negatively correlated with ammonium-nitrogen and total phosphorus in structural equation model, was a dominant factor influencing water quality. These findings will help us to better understand the factors of controlling rural domestic sewage discharge at a national scale and to optimize the treatment technology of rural domestic sewage.

- **Keywords:** Rural domestic sewage; Water quantity; Water quality; Water resources; Gross domestic product; Structural equation model

Xiaoyan Liu, Hao Guo, Xinying Zhang, Shenyu Zhang, Xinde Cao, Ziyang Lou, Wei Zhang, Zhiqun Chen. *Modeling the transport behavior of Pb(II), Ni(II) and Cd(II) in the complex heavy metal pollution site under the influence of coexisting ions*. Pages 211-218.

Complex metal contaminated sites are generally more harmful than single metal contaminated sites. Therefore, this study combined experiment and mathematical model to investigate the migration of Pb(II), Ni(II) and Cd(II) in single and multi-metal systems. The data from batch and column experiments were fitted well by Langmuir and nonequilibrium convection-dispersion equation. In the single metal system, the adsorption capacity of metals in soil was Pb> >Cd>Ni. In multi-metal systems, Pb(II), Ni(II) and Cd(II) retention in column decreased by 42.8%, 56.2% and 92.8% respectively due to the competition effect. The competitive effect enhanced the migration of three metals in the column. Ni(II) and Cd(II) showed irregular breakthrough curves, called "overshooting", under the effect of Pb(II). The phenomenon of overshooting made the outlet concentration C of the column greater than the inlet concentration C0 (C/C0>1), leading to serious potential risks to groundwater. In addition, results from speciation of metals showed that the competition effect and overshooting mainly occurred in exchangeable and carbonate fractions. Understanding the transport of metals in complex contaminated sites is important for risk assessment.

- **Keywords:** Breakthrough curves; Competitive effect; Soil column; Speciation of metals; Transport

Li Dai, Minjie Shan, Jianping Li, Jianqi Chen, Wenjie Lv, Pengbo Fu, Hongpeng Ma, Hualin Wang. *Purification and reuse of carbon black wastewater of acetylene production from natural gas by microchannel filtration*. Pages 219-229.

Carbon black wastewater is a by-product of partial oxidation of natural gas to acetylene and can cause serious pollution to the environment. In this study, the effect of deep bed filtration (microchannel filtration) in the synergistic separation of particulate pollutants and organic pollutants in carbon black wastewater were investigated. The results indicated that the separation efficiency of carbon black particles with a mean diameter of 6.88 μm was 95%– 98%, 95–97%, and 95%– 96% when the filter material was quartz sand + quartz sand, quartz sand + activated, and quartz sand + anthracite, respectively. The solid content of inlet was 300 mg/L and 145 NTU, respectively, and those of the purified effluent were below 15 mg/L and 14 NTU, which meet the first-class B standard of China sewage discharge. The total kinds of organics were reduced from 29 to 2. The separation efficiency of C6-C24 all higher than 97%. A 150 m3/h full-closed treatment process for carbon black wastewater was designed to replace the original open sedimentation tank. The carbon black wastewater could be efficiently purified by this method, the purified carbon black wastewater could be reused, and the carbon black was used to make a filter cake for recycling in rubber without discharge. Finally, the possibility of achieving zero discharge of carbon black wastewater is shown.

- **Keywords:** Acetylene production; Carbon black wastewater; Microchannel filtration; Purification

S.C. Chakraborty, M. Qamruzzaman, M.W.U. Zaman, Md Masruck Alam, Md Delowar Hossain, B.K. Pramanik, L.N. Nguyen, L.D. Nghiem, M.F. Ahmed, J.L. Zhou, Md. Ibrahim.H. Mondal, M.A. Hossain, M.A.H. Johir, M.B. Ahmed, J.A. Sithi, M. Zargar, Mohammad Ali Moni. *Metals in e-waste: Occurrence, fate, impacts and remediation technologies*. Pages 230-252.

Electronic waste (e-waste) is generated from the discarded electronic products. The generation of e-waste has increased significantly in the recent decades. Globally, the increased rate of e-waste generation is almost 2 metric tonnes (Mt) per year. It is estimated that about 74 Mt of e-waste will be produced in 2030. Therefore, e-waste can be a significant threat to the environment. Toxic metals (e.g., lead, mercury, nickel, and cadmium) are released to the environment from the e-waste and eventually enter into soil, sediment, groundwater, and surface water. The release of toxic metals in the environment causes adverse effects on human health, aquatic animals, and plants. Therefore, the proper management of e-waste is essential and becomes a major concern in the world. In this regard, this review provides a comprehensive summary of the occurrence, fate, and remediation of metals generated from e-waste. The literature survey revealed that household electrical appliances are the primary source of e-waste, comprising approximately 50% of the overall production of e-waste. Among different remediation technologies, the combination of biological, physical, and chemical processes shows relatively high removal efficiency; and they possess multiple advantages over other remediation technologies. Finally, this review also includes future outlook on e-waste management and remediation technologies.

- **Keywords:** E-waste; Metals; Bioavailability; Accumulation; Remediation; Hybrid

Chandrabhan Verma, Mumtaz A. Quraishi, K.Y. Rhee. *Natural ligands: Promising ecofriendly alternatives for corrosion protection and plethora of many prospects*. Pages 253-290.

Natural ligands are the naturally existing chemicals that are extracted from plants and animals without further modification. For the reason that of their biotic and natural invention, these supplies can be treated as green and sustainable replacements for traditional ligands as they are fairly harmless, nonbioaccumulative and biodegradable. Currently, the growing demands of green chemistry and sustainable development inspire the growth and use of these materials and their chemically modified derivatives. Literature search advises that these materials possess widespread of biological and industrial applications. In the present review, coordination bonding ability of some main series of natural ligands including amino acids, proteins, carbohydrates, polyphenols, flavonoids, fatty acids, oleochemicals, purines and pyrimidines, drugs and phytochemicals in correlation with their corrosion protection effectiveness and with possibility of other uses is reviewed, described and proposed. Herein, the advantages of natural ligands and disadvantages of traditional ligands along with future perspective and research gap is described. Obviously, natural ligands contain many electron rich sites in their molecular structure that help them in binding with metal surface effectively. The natural ligands generally form chelating complexes with the metal atoms or ions. Because of their complex formation ability, these ecofriendly ligands can also be used to replaced traditional toxic ligands being used for other applications such as metal decontamination, ion exchange, wastewater and industrial influents treatments.

- **Keywords:** Natural ligands; Coordination bonding; Chelating complex; Coordination polymers and Corrosion protection

Xiaolu Yue, Yuwen Wang, Qi Zhou, Yang Lyu, Ying He, Zhenwu Tang. *Phthalates in soil and road dust from a large processing trade center of children's clothing: Occurrence, profiles and potential health risks*. Pages 291-300.

Phthalates have been frequently used in various clothing as plasticizers. However, little information is available on phthalates in the environmental matrices in clothing processing sites. This study investigated the phthalates in the soil and road dust in a large processing trade center of children's clothing in China based on the characteristics of human activities and regional environment. The total concentrations of 13 phthalates were in the range of 219–15,952 and 1104–18,628 ng/g, respectively. We did not find extremely high concentrations of phthalates, and our reported concentrations were moderate in comparison with those reported in other areas. Bis(2-ethylhexyl)phthalate was the dominant congener, representing medians of 64.3% and 77.4% of the total phthalate concentrations in the soils and road dust, respectively. Source assessment suggested that the phthalates were likely mainly from the processing process of clothing, and some may have been originated from the use of family products. The health risk assessment results showed that the risks from phthalates in the soils and road dust were generally low. However, more research is required to investigate the phthalate contaminations and the associated risks due to the lack of relevant information in textile industrial areas.

- **Keywords:** Garment processing; Environmental matrices; Plasticizers; Distribution; Environmental exposure

Linlin Zhang, Jiansong Wu, Jun Zhang, Feng Su, Haifeng Bian, Long Li. *A dynamic and integrated approach of safety investment decision-making for power grid enterprises*. Pages 301-312.

Recently, the consequences caused by frequent large-scale power grid accidents are more significant with arousing great attention of power grid enterprises. Scientific safety investments are essential to improve the overall safety level of the power grid enterprises and promote safe production. This study proposed a dynamic and integrated approach for safety investment decision-making of power grid enterprises based on the entropy weight method (EWM) and the system dynamics (SD) theory. By applying the accident loss assessment and the safety performance evaluation, the SD-based model for the safety investment decision-making for power grid enterprises was developed. The results show that risk assessment is the critical factor for power grid safety, followed by safety training, organizational investment, and technological investment. Moreover, the proposed safety investment decision-making model can be continuously updated and optimized with future emerging data to support the dynamic prediction of power grid safety investment.

- **Keywords:** Power grid enterprises; Safety investment; System dynamics; Accident loss

Injun Kim, Jinwon Park, Yunsung Yoo. *Formation and polymorph transformation trends of metal carbonate in inorganic CO2 conversion process using simulated brine: Study for post-treatment of industrial brine via CO2 conversion*. Pages 313-327.

To improve inorganic carbon capture utilization (CCU) technology, practical solution for global warming technology, we studied the formation and transformation trends of mineral carbonation using simulated brine. we converted CO2 into inorganic compounds, metal carbonate, using CO2 saturated aqueous monoethanolamine (MEA) solution. The produced metal carbonate varied according to the simulated brine's cation component,

resulting from ion interactions in the system. It turns out that the common ion effect, which occurred due to the system's ion interactions involving changes of ionic atmosphere and salinity of the system, was the main reason for the various carbonation trends. Salting- out effect dominantly occurred in the single precipitation system whereas salting-in effect occurs in multi precipitation system (system CM and system CMN). However, salting-out effect also occurred in system CMN because of Na+. Moreover, we also found that Na+, which was overlooked in prior studies regarding polymorph transformation, also affects polymorph transformation. The interactions between the abovementioned effects involved the variation in the results. This variation interrupted the wide usage of the technology. However, through the study, we suggest ambient estimation of the final product with cation component. It would help future studies and demonstration of the inorganic CCU technology using brine.

- **Keywords:** Climate change mitigation technologies; Carbon capture utilization(CCU); CO2 utilization; Inorganic CO2 conversion; Mineral carbonation; Metal carbonate

Yubo Bi, Zhian Yang, Haiyong Cong, Mingshu Bi, Wei Gao. *Experimental and theoretical investigation on the effect of inclined surface on pool fire behavior*. Pages 328-336.

Potential pool fire hazards due to the leakage of combustible liquid chemical materials during storage and transportation pose a threat to process safety in the process industry. A pool fire may occur on the inclined surface of broken pipelines or facilities. The influence of an inclined surface on pool fire behavior was experimentally and theoretically studied. The results showed that the flame tilt angle and flame length increased with inclination angle, while the flame height exhibited an opposite trend. These phenomena were mainly caused by the restriction of air entrainment due to the inclined surface. The flame pulsation frequency generally decreased with the increase of inclination angle and was weakly dependent on the heat release rate. Dimensionless models were developed to predict the flame tilt angle, flame length, flame height, and flame pulsation frequency. The predictive values were in good agreement with experimental data.

- **Keywords:** Inclined surface; Flame tilt angle; Flame length; Flame height; Flame pulsation frequency

Zahid Ullah, Muzammil Khan, Salman Raza Naqvi, Muhammad Nouman Aslam Khan, Wasif Farooq, Muhammad Waqas Anjum, Muhammad Waqas Yaqub, Hamad AlMohamadi, Fares Almomani. *An integrated framework of data-driven, metaheuristic, and mechanistic modeling approach for biomass pyrolysis*. Pages 337-345.

This study presents an integrated hybrid framework of data-driven (cascade forward neural network (CFNN)), metaheuristic (artificial bee colony (ABC)), and a mechanistic modeling (Aspen simulation) approach for the biomass pyrolysis process for bio-oil production. We applied CFNN and an ABC to predict and optimize bio-oil yield. The CFNN model achieved high prediction performance with a correlation coefficient value of 0.95 and a root mean squared error value of 0.39. Furthermore, the CFNN-ABC derived optimum parameters were then validated using a mechanistic model of the pyrolysis process. The CFNN and Aspen simulation results were following the experimental results, with an average deviation of 5%. The feature importance showed that the internal information about biomass was more relevant than external factors for bio-oil yield. The partial dependence plots were developed to know the insights into the biomass pyrolysis process. This study presents a modeling and simulation platform for bio-oil production that can increase the waste-to-energy process and can be helpful for academia.

- **Keywords:** Biomass; Bioenergy; Machine learning; Cascade neural network; Artificial bee colony; Aspen plus

Yaxuan Xiong, Chaoyu Song, Jing Ren, Yuhe Jin, Binjian Nie, Qian Xu, Yuting Wu, Chuan Li, Haimeng Li, Yulong Ding. *Sludge-incinerated ash based shape-stable phase change composites for heavy metal fixation and building thermal energy storage*. Pages 346-356.

Incineration is a harmless way to treat municipal sludge. However, it is difficult to fix heavy metals in the sludge-incinerated ash (SIA). To fix the heavy metals and recycle the SIA effectively, this work innovatively proposed the SIA as skeleton material, and five shape-stable phase change composites (SSPCCs) with different mass ratios of SIA to NaNO3 (phase change material, PCM) were fabricated via the cold-compression & hot-sintering (CCHS) method. Then, key thermal performance, mechanical strength, and micromorphology were investigated while the chemical compatibility between the SIA components and NaNO3 was analyzed. Results showed that the SSPCCs could fix the heavy metals properly, and the SIA was suitable for skeleton material; The SSPCC with the mass ratio 5:5 of SIA to NaNO3 reached a maximal thermal energy storage (TES) density of 409.25 kJ/kg in the range of 100–400 °C, which had high mechanical strength of 139.65 MPa and good thermal stability; The SIA components demonstrated excellent chemical compatibility with NaNO3.

- **Keywords:** Municipal waste recycling; Skeleton materials; Thermal energy storage; Thermal stability; Chemical compatibility

Zhuang Li, Shenping Hu, Xiaoming Zhu, Guoping Gao, Chenyang Yao, Bing Han. *Using DBN and evidence-based reasoning to develop a risk performance model to interfere ship navigation process safety in Arctic waters*. Pages 357-372.

Risk performance reasoning strategy for LNG ships navigating in Arctic waters is proposed in this paper. Many uncertainties exist in the reasoning of ship navigation risk in Arctic waters, which are influenced by multi-source risk causing events. As a result of the aforementioned concerns, the dynamic Bayesian network (DBN) structure is offered as a solution for an uncertain risk assessment model. The DBN network can benefit from a strategy for solving ambiguous data information based on Dempster–Shafer (D–S) evidence theory and a cloud model. Additionally, a risk performance reasoning technique for LNG tanker collision accidents in Arctic waters is developed. Besides, the marine meteorological reanalysis data, data from ship-borne sensor monitoring, and expert knowledge in the suggested risk performance reasoning method are incorporated. A case study confirmed that the risk performance reasoning of accidents was needed revealed that the main risk in Arctic summer waters is posed by obstacles in the channel that are difficult to detect, such as icebergs and reefs.

- **Keywords:** Risk performance reasoning; Dempster–Shafer evidence theory; Dynamic Bayesian network; Cloud model; Arctic waters

Miao Gong, Mengqi Wang, Linlu Wang, Aixin Feng, Jinxiang Hu. *Degradation of tetracycline hydrochloride in sub- and supercritical water with and without oxidation*. Pages 373-383.

In the present work, in a batch quartz tube reactor, supercritical water gasification and supercritical water oxidation were used to treat tetracycline hydrochloride (TC). The results show that the increase in temperature, the extension of reaction time, and the decrease in initial concentration all had a positive impact on the removal of TC. After adding 0.108 mol/L H2O2 (n = 1), the removal rate reached 100% at 1000 mg/L, 400 °C

and 100 s. First-order degradation kinetics was used to fit the degradation of TC. In the absence of H2O2, its pre-exponential factor and activation energy were found to be 0.03 s−1 and 6.14 kJ/mol, respectively. After adding H2O2, its pre-exponential factor and activation energy were found to be 6.70 s−1 and 25.66 kJ/mol, respectively. The degradation process of TC was explored and the results show that TC can be degraded into smaller molecular substances in supercritical water. After adding H2O2, the degradation efficiency of TC was significantly improved the degradation process was also more thorough. There were two main degradation processes, namely the ring-opening reaction and the central carbon cracking.

- **Keywords:** Tetracycline hydrochloride; Supercritical water; Oxidation; Kinetics; Degradation mechanism

Xinyu Chang, Chunhua Bai, Bo Zhang. *The effect of gas jets on the explosion dynamics of hydrogen-air mixtures*. Pages 384-394.

In the real scenarios, explosions generally occur under turbulent environments. In this study, the turbulence is generated by introducing inert gas jets, and the interaction between jet turbulence and inert gas dilution is extremely complicated under different conditions. Therefore, the aim of this study is to investigate the influence of gas jets on explosion behavior of hydrogen-air mixtures with various hydrogen concentrations (from 10% to 70%) at different initial pressures (i.e., 50 kPa, 100 kPa, 150 kPa, 200 kPa), and a series of experiments are conducted in a standard 20 L spherical explosion chamber at environmental temperature 300 K. The effect of gas jets on explosions of hydrogen-air mixtures with various hydrogen concentrations at initial pressure of 100 kPa is first studied, the experimental results illustrate that jet has minor impact on the explosion behavior when hydrogen concentration ranges from 20% to 70%. However, the enhancement effect of gas jets on the reaction process is significant as hydrogen concentration is 10%. Therefore, the impact of various gas jets (i.e., CO2, and N2) on explosion behavior at different initial pressure is mainly examined as hydrogen-air mixtures are near the lower explosive limits. It is found that the enhancing effect of gas jets on explosion behavior is profound for hydrogen-air mixtures at higher initial pressure, however, the suppression effect caused by the higher concentration of inert gas could balance the promoting effect by turbulence at lower initial pressure. Moreover, the encouraging effect of CO2 jet is more apparent than that of N2 jet when jet duration time is relatively short, because the turbulence intensity induced by CO2 is greater due to its larger molecular weight.

- **Keywords:** Hydrogen-air mixtures; The flame propagation speed; Gas jets; Explosion

Chao Liu, Wei Luo, Zehai Liu, Jie Long, Subei Xu, Hongwei Liu, Xuegang Wang. *Microwave absorption properties of spent green phosphor and enhanced extraction of rare earths*. Pages 395-405.

The efficient extraction of rare earth elements from spent phosphor was achieved by microwave alkali fusion -leaching. Effect of temperature on the dielectric properties was studied. The addition of alkali greatly enhanced the microwave heating ability of the phosphor with loss tangent value increasing from 0.031 to 0.084 at 800 °C, which was ascribed to the strong susceptibility of molten sodium hydroxide and roasted products to microwave interaction. Effects of process parameters of roasting and acid leaching were investigated. When the phosphor was treated at 800 °C for 30 min with mass ratio of NaOH/phosphor of 2:1 followed by acid leaching of 4 mol/L HCl with the liquid-solid ratio of 10:1 at 60 ºC for 120 min, the leaching efficiencies of Ce and Tb were 97.86% and 95.75%, respectively. Microwave roasting showed the advantages of lower temperature, shorter time and higher leaching ratio of rare earths compared with conventional roasting. Enhanced thermal motion of sodium hydroxide, improved kinetic conditions and

changes of crystal structures resulting from microwave selective heating may be responsible for microwave-enhanced rare earths extraction. Kinetic studies showed that both the alkali roasting and leaching process of rare earths were controlled by product layer diffusion.

- **Keywords:** Microwave roasting; Dielectric properties; Phosphor; Rare earth; Kinetics

Safaa Khattabi Rifi, Salah Souabi, Loubna El Fels, Anas Driouich, Ilham Nassri, Chaymae Haddaji, Mohamed Hafidi. *Optimization of coagulation process for treatment of olive oil mill wastewater using Moringa oleifera as a natural coagulant, CCD combined with RSM for treatment optimization*. Pages 406-418.

Wastewater from olive oil mills (OMW) represents a major environmental problem that requires effective treatment to decrease pollution. In the present work, the treatment of olive oil mill wastewater by coagulation was studied using Moringa Oliefera as a natural coagulant. The processing is optimized using both Design of Experiments (DOE) methodology and a central composite design (CCD) combined with the response surface methodology (RSM). The optimization describes the relationship between 3 responses (turbidity, COD, and polyphenols) and 4 independent variables (Moringa Oliefera concentration, pH, agitation speed, and time). Analysis of variance ANOVA using Fisher's test indicated that the established models were significant. The study showed that the model was characterized by a good fit, justified by the very high adjusted coefficient of determination (R2Adj = 86.73%, R2Adj = 90.39% and R2Adj = 93.33% for the turbidity, COD, and polyphenols, respectively). Furthermore, the optimum conditions for a good purification performance of OMW using Moringa Oliefera are as follows [Mo] = Moringa Oliefera = 65 g/L, pH = 6, Agitation speed (Ss) = 35 rpm and Agitation time (St) = 25 min. Under these conditions, the turbidity, COD and polyphenol removal efficiencies are 96%, 88%, and 86% respectively. Finally, the proposed treatment process is a critical development in sustainable environmental technologies.

- **Keywords:** Olive mill wastewater; Optimization process; Response surface methodology; Moringa oleifera; Centered composite plan

Fallah Hashemi, Hassan Hashemi, Alireza Abbasi, Madeline E. Schreiber. *Life cycle and economic assessments of petroleum refineries wastewater recycling using membrane, resin and on site disinfection (UF-IXMB-MOX) processes*. Pages 419-425.

The use of treated effluent as a sustainable, reliable, and accessible source of water supply is a critical factor influencing water use in industrial sectors like petroleum refineries. The purpose of this study is to document the life cycle and economic assessment of an integrated ultrafiltration, ion exchange, and multioxidant (UF-IXMB-MOX) treatment system in the recycling of refinery effluent. The effluent was used to supply makeup water in cooling towers at the Kermanshah oil refinery, Iran from April to December 2018. For the life cycle analysis, eight environmental indicators, including ozone-depleting potential (ODP), global warming (GW), greenhouse gases (GHG), acidification potential (AP), eutrophication potential (EP), health effects (HE), environmental toxicity potential (ETP) and photochemical oxidation potential (POCP) were considered for four groups influencing the selection of a treatment method, including electricity consumption (EC), raw materials, condensed effluent (concentrate) and construction. Results of the economic analysis show that the initial investment for the launch of this treatment system was estimated at $255,750. Considering the fixed and variable annual costs, the cost of regenerating treated effluent was estimated at $0.24/m3 of effluent, with the cost of chemicals contributing the most to annual costs.

This scenario, with consumption of 0.08kWh/m3, had the lowest energy consumption compared to other similar membrane-based methods. The electricity consumption in the formation of GHGs, GW, POCP, and health effects, and the role of condensed effluent produced in creating ETP in aquatic and terrestrial environments, had the highest environmental impact among the eight environmental indicators. Overall, results suggest that focusing on renewable energy and the use of chemicals with minimal economic and environmental impact can increase the efficiency of this process.

- **Keywords:** Oil Refinery; ZLD; Effluent Recycling; LCA

Xiaodong Tian, Lanxin Xie, Yaoshan Li, Yuan Liu, Songbo Ma, Dehong Kong, Xianwen Zhu. *Green process for recovering indium and other precious metals from high-sulphur hot filter residues via sodium-hydroxide hydrothermal treatment*. Pages 426-434.

Indium (In) has vital applications in solar photovoltaic technology and light-emitting diodes. However, the resource for In production is low. Zinc smelting is an important source of In, but the average In recovery rate is only 20%. The annual economic loss due to the loss of In is as high as USD 199.7 million. In this study, a high-sulphur hot filter residue (HFR) was processed via sodium-hydroxide (NaOH) hydrothermal treatment (NAHT). By varying the amount of NaOH and using the dissolution exotherm of NaOH, sulphur element (S0) in HFR was transferred to a liquid phase. Thus, In and other precious metals originally wrapped in S0 were enriched in the slag phase (TLR). The In grade in TLR was as high as 1700 g/t, and the recovery rate was 99%. In addition, 10.94 g/t gold, 125.81 g/t silver, 15.18% zinc and 22.27% iron were incidentally recovered. The wastewater produced in the process showed better effects than industrial Na2S in flotation processes. Thus, NAHT is an effective green recovery technique for recovering In and other precious metals from HFR. Further, the recovered In can yield an annual revenue of USD 1,122,170 for the plant. Therefore, the treatment of HFR plays an important role in zinc hydrometallurgical smelting plants.

- **Keywords:** Indium; Hot filter residue; Hydrothermal treatment; Green technology; Resource reuse; Sustainability

Dadi V. Suriapparao, Ravi Tejasvi. *A review on role of process parameters on pyrolysis of biomass and plastics: Present scope and future opportunities in conventional and microwave-assisted pyrolysis technologies*. Pages 435-462.

Pyrolysis is one of the thermochemical conversion platforms for biomass and plastics into value-added product resources. The products formation significantly varied with feedstock composition, pyrolysis parameters, and heating source. Hence, the objectives of this review article are to understand the role of type of feedstock, heating rate, reaction temperature, residence time, feedstock particle size, and type of pyrolysis reactor. In addition, the upgradation of bio-oil using physical and catalytic approaches has been analyzed. Co-pyrolysis and catalytic co-pyrolysis which promote the product properties through synergy are also investigated. The role of microwave heating with the help of a susceptor to promote product synthesis is discussed. The metal oxide and zeolite catalysts' role in the formation mechanism of hydrocarbons and oxygenates are studied. For the future scope, the studies related to pyrolysis-combustion combination, microwave hybrid heating, and continuous catalytic co-pyrolysis are promising approaches. To this end, this review bridges the research gap in the domain of pyrolysis process parameters, and waste valorization using microwave-assisted pyrolysis, co-pyrolysis, and catalytic co-pyrolysis technologies. Moreover, this review would further provide the way for the current issues related to effective biomass and plastic waste utilization.

- **Keywords:** Biomass; Plastics; Pyrolysis; Microwave; Co-pyrolysis; Bio-oil

V. Shenbaga Muthuraman, Adamya Patel, Vemuluri Shreya, Avinash Vaidyanathan, K.N.G.L. Reshwanth, C. Karthick, Michal Jan Gęca, B. Ashok, K. Sivagami, K. Nanthagopal. *Progress on compatibility issues of alcohols on automotive materials: Kinetics, challenges and future prospects- a comprehensive review*. Pages 463-493.

Alcohol could be the biggest factor in the improvement of the world biofuel economy in the present century due to its excellent properties on par with petroleum products. The biggest concern in the commercialization of alcohols is their material compatibility issues with various metals due to acidic form, moisture absorption and oxygenated nature. This review has been made to summarize the operational difficulties of alcohol for automotive applications. In the first phase of the review, the chemical kinetics of alcohols on corrosive formations has been outlined. In the second phase of the review, the effect of low carbon alcohols on various metals that were used in automotive engines and the compatibility issues were discussed in detail. Further, the study has been outlined microbiologically induced corrosion (MIC) of metals. Several limitations of alcohol usage with automotive engine components are highlighted and possible remedies are also recommended for corrosion reduction. In the end, special attention has been on various corrosive inhibitors for alcohol applications with a variety of materials. The properties like diffusion, acidity, conductivity and electro-potential are more dominant factors in corrosive formation. The comprehensive review shows that the oxygenated form and moisture absorption ability are the pivotal factors in the material compatibility of alcohols. The studies are also recommended that butanol has better anticorrosive qualities among all alcohols due to its less affection for water. Further, it is also identified that polymer-based materials and high-density polyethylene are the most appropriate materials for alcohol-based fuel supply systems and proper concentration of corrosion inhibitors with alcohols is of high importance for long-term application also. Several possibilities for the improvement of materials compatibility of all alcohols are also suggested.

- **Keywords:** Biofuels; Alcohols; Material compatibility; Corrosion; Corrosion inhibitors

A.O. Zhdanova, R.S. Volkov, G.V. Kuznetsov, N.P. Kopylov, S.N. Kopylov, E.Yu. Syshkina, P.A. Strizhak. *Solid particle deposition of indoor material combustion products*. Pages 494-512.

Heavy smoke emission during fires hampers evacuation of people and movement of rescue teams to a fire source. It is often pyrolysis and combustion products that cause deaths from fires in closed spaces. Fire sprinkler system activation does not always lead to efficient smoke deposition. Sometimes, a fire suppression liquid supply, on the contrary, deteriorates fire evacuation conditions. The study of smoke generation and deposition characteristics is an essential prerequisite for improving rescue technologies during fires. The purpose of this research was to define the characteristics of deposition of solid combustion product particles of a group of typical construction and finishing materials in closed spaces: wood, linoleum, rubber, etc. Solid particles (pyrolysis products) have been distributed by size and concentration. The smoke generation and extinction coefficients, as well as deposition rates of smoke aerosol particles with and without using water aerosol have been determined. The ranges of optical properties of smoke aerosol have been specified. The time of dispersed water impact on smoke aerosol was varied to evaluate its effect on the mass rate of deposition of solid combustion product particles. The characteristics of absorption of laser radiation with different wavelengths in flue gases have been defined to identify the most advantageous colors of

reflector materials used to manufacture direction signs for the evacuation of people from the combustion zone.

- **Keywords:** Compartment fires; Combustion products; Smoke emission; Smoke deposition; Capture of solid particles; Aerosol wetting

Yin Wang, Shang-Hao Liu, Chin-Lung Chiang, Li-Yu Zhang, Wen-Tao Wang. *The effect of oxygen on the thermal stability and decomposition behaviours of 1,3-dimethylimidazolium nitrate for application using STA, ARC and FTIR*. Pages 513-519.

The thermal decomposition and runaway reaction of 1,3-dimethylimidazolium nitrate ([Mmim]NO3), a typical nitrate IL, were studied by a simultaneous thermogravimetric analyzer (STA) and accelerating rate calorimeter (ARC). The STA results show that the thermal decomposition of [Mmim]NO3 is divided into two stages, and the decomposition behaviour is similar in nitrogen or oxygen. The experimental results under adiabatic conditions indicate that [Mmim]NO3 has higher Tmax and Pmax than other imidazolium ILs, which reflects the greater explosion hazard of [Mmim]NO3. The apparent activation energies of [Mmim]NO3 were 86 kJ/mol and 83 kJ/mol, as calculated by the F-W-O and K-A-S methods. The complete thermal decomposition gas products of [Mmim]NO3 were analyzed by thermogravimetry coupled with Fourier transform infrared spectroscopy (TG-FTIR), and the gas released by thermal decomposition of [Mmim]NO3 does not react with oxygen. Therefore, the decomposition reaction of [Mmim]NO3 was not positively related to the concentration of oxygen, which indicated that [Mmim]NO3 could play an active role in the reactions in the presence of oxygen. The results of this study may provide theoretical and experimental basis for [Mmim]NO3 safety precautions in storage and transportation.

- **Keywords:** Decomposition behaviours; Thermal hazards; Nitrogen or oxygen; Thermogravimetric analyser-FTIR spectrometer; 1, 3-dimethylimidazolium nitrate ([Mmim]NO3)

Juliana Mendonça Silva de Jesus, Flávio Kiyoshi Tominaga, Allan dos Santos Argolo, Ana Cristina Gomes Nascimento, Sueli Ivone Borrely, Daniel Perez Vieira, Daniele Maia Bila, Antonio Carlos Silva Costa Teixeira. *Radiolytic degradation of levonorgestrel and gestodene: Performance and bioassays*. Pages 520-530.

This study reports the feasibility of ionizing sources (60Co source and electron beam radiation) to degrade the progestins hormones levonorgestrel (LNG) and gestodene (GES) in synthetic solutions and real pharmaceutical wastewater (RPW). Doses of 0.5–100 kGy and dose rates of 2.5 and 10 kGy h−1 were applied. LNG was shown to be more recalcitrant than GES, with 90% removals achieved at doses around 7.7 kGy (LNG) and 1.6 kGy (GES) in model systems, with LNG showing greater reactivity with reducing species in γ-radiolyis, unlike GES. Furthermore, LNG removal remained around 60% in RPW at low doses, while more than 60% GES removal was observed for all doses. LNG and GES toxicities to Daphnia similis were absorbed dose-dependent, with low doses resulting in toxicity reductions of around 32% (LNG) and 42% (GES); in turn, high doses promoted a fourfold increase in toxicity. γ-radiolysis reduced the cytotoxic character of LNG to NIH-3T3-L1 cells, while non-irradiated or irradiated GES solutions did not exhibit any cytotoxic effect. Finally, the estrogenic activity, evaluated by the YES assay, was dose-dependent for both progestins, which may be related to the evolution of transformation products formed by water radiolysis in each case, decreasing for high doses.

- **Keywords:** Progestins; Pharmaceutical wastewater; Gamma-rays; Electron beam; Water radiolysis

Peizhen Chen, Xiangqun Zheng, Weimin Cheng. *Biochar combined with ferrous sulfate reduces nitrogen and carbon losses during agricultural waste composting and enhances microbial diversity*. Pages 531-542.

This study investigated the effects of adding biochar, ferrous sulfate, and their combination during composting of pig manure mixed with straw to reduce the loss of carbon and nitrogen during agricultural waste composting. Four 100 L fermentation tank-scale experimental composting treatments were established: the additive-free control (CK), addition of 5% biochar (BC), addition of 5% ferrous sulfate (SF), and addition of 2.5% BC + 2.5% SF (BS). The transformation of carbon and nitrogen and the change characteristics of bacterial communities during composting of the four treatments were explored. BS significantly reduced NH3, N2O, CO2, and CH4 emissions by 59.57%, 48.41%, 35.80%, and 32.25% compared with CK, respectively. The BS treatment showed lower carbon and nitrogen losses than the single additive treatment. BS treatment enhanced the diversity and richness of bacterial communities during composting. The redundancy and Pearson correlation analyses revealed that the composition of dominant species between treatments had significant differences in different compost periods (mesophile, thermophilic, and cooling periods). BS treatment significantly increased the abundance ratio of carbon sequestration and nitrogen retention communities, and it enhanced nutrient preservation by microbial metabolism. Therefore, the composite addition of biochar and ferrous sulfate is an effective method to reduce the loss of carbon and nitrogen during agricultural waste composting.

- **Keywords:** Compost; Agricultural waste; Nitrogen loss; Carbon loss; Bacterial community

Zhiqiang Cao, Binggan Wei, Linsheng Yang, Jiangping Yu, Min Meng, Qing Chen, Feng Li. *Different crop rotation patterns vary heavy metals behavior in soils under plastic sheds: Evidence from field research*. Pages 543-552.

Facility agriculture improves food supply worldwide. However, heavy metals accumulation in its soils under plastic sheds increases the contamination risk, and little is known about metal's behavior in soils under different rotation patterns. This study investigated total and available Cd, Cu, Ni, Pb, and Zn in soils under plastic sheds from tomato-cropping (TCC), tomato-leaf vegetable rotation (TVC), tomato-melons rotation (TMC), and fruit-cropping (FLC). Results indicated that accumulations and bioavailability of Cd, Cu, and Zn were severe, and risks of tomato-based rotations were higher than FLC. Geo-accumulation index showed that accumulation of Cu and Zn in soils from TCC was the worst, and Cd in TVC was the highest. Principle-component analysis suggested Cu and Zn might be from manures. Linear regression analysis showed significant annual increases of total Cu and Zn in TCC; Cd in FLC and available Cd in TVC should be taken seriously. Different fertilizers and dry matter removal might be reasons for different behaviors of metals. The lowest amounts of both factors in FLC make its soils healthier. Tomato-based patterns should consider more intercropping and rational fertilization, and FLC might be an alternative. Proper fertilization and selection of rotation patterns can prompt soil health of facility farmlands.

- **Keywords:** Soil security; Heavy metals; Facility agriculture; Crop rotation

Jusong Kim, Jinwon Yu, Chollyong Kang, Gwangil Ryang, Yanjie Wei, Xiaoli Wang. A novel hybrid water quality forecast model based on real-time data decomposition and error correction. Pages 553-565.

Accurate forecast for water quality is of great importance because it can support water resource management with the future information. In this research, we propose a novel hybrid model by using data decomposition, error correction, and machine learning. In our method, first, the initial forecast is obtained by a prediction model that uses improved complete ensemble empirical mode decomposition with adaptive noise and bidirectional long short-term memory (BLSTM) neural network. Next, a novel error correction framework, which is built by variational mode decomposition and BLSTM neural network, is used to improve forecast accuracy by correcting the initial forecast error. Water quality data of Poyang Lake, China is used to evaluate our model. Results indicate that our model shows highly accurate forecast performance for all of the 9 water quality datasets (the average of mean absolute percentage error (MAPE) of 7 day-ahead forecast is 2.12%; 30 day-ahead forecast is 4.06%). In addition, our model outperforms the competitor models, particularly, compared to the prediction model without error correction framework, the average of MAPE is reduced by 33.33% for 7 day-ahead forecast; 30.48% for 30 day-ahead forecast. This research demonstrates that the proposed error correction framework is an effective tool to improve forecast accuracy for water quality.

- **Keywords:** Water quality; Hybrid model; Machine learning; Improved complete ensemble empirical mode decomposition with adaptive noise (ICEEMDAN); Bidirectional long short-term memory (BLSTM); Variational mode decomposition (VMD)

Saeed Nazari, Roonak Daghigh. *Techno-enviro-exergo-economic and water hygiene assessment of non-cover box solar still employing parabolic dish concentrator and thermoelectric peltier effect*. Pages 566-582.

This study was conducted to design a parabolic dish concentrator box solar still without a glass cover combined with a thermoelectric condensing duct. The parabolic set reflects the sun's rays beneath the basin and the vapor generated in the basin is sucked by a fan with variable volume flow rate into the condensing duct, which is surrounded by four thermoelectrics cooling modules. The performance of non-cover box solar still with thermoelectric is reported based on the component temperature, distilled water production, energy, exergy, energy payback period, energy production factor, economic, exergoeconomic, environmental, enviroeconomic, exergoenvironmental, exergoenviroeconomic, and water hygiene assessment. In the optimal case, in which the fan sucks the vapor at a volume rate of 300 L/min, the average winter daily cumulative distilled water, energy efficiency, and exergy efficiency were enhanced by 25.6%, 4.88%, and 1.06%, respectively, compared to the case, which the fan is off. The cost of distilled water production and the payback period in the optimal case are 0.0056 $/L/m2 and 114 days, respectively. Also, the techno-enviro-exergo-economic findings revealed that the parabolic dish concentrator box solar still with thermoelectric in terms of enviroeconomic and exergoenviroeconomic can create a financial reserve of $320.02 and $50.32, respectively. The distilled water produced by the desalination system is safe in terms of hygiene and drinking ability.

- **Keywords:** Non-cover box solar still; Parabolic dish concentrator; Thermoelectric condensing duct; Techno-enviro-economic; Water hygiene assessment

Goh Choo Ta, Noorazman bin Soud, Kasman bin Nasir, Fairuz Anwar bin Abdullah, Masli Irwan Rosli, Darman Nordin, Jarinah Mohd Ali, Syazwani Binti Mohd Fadzil, Nurul Izzaty Binti Hassan, Siti Zubaidah Hasan, Mohd Sobri Takriff, Mardiana bt. Abdul Latif. *Prevention of technological disasters: Adoption of indicative criteria associated with GHS in regulating major accident hazards*. Pages 583-594.

The occurrence of a technological disaster could be due to different causes, one of which is chemicals. The major accidents triggered by chemicals, such as the Seveso incident in 1976, the Bhopal incident in 1984, and the recent Beirut explosion in 2020, have had severe impacts on people and the environment. Many countries have established their respective regulatory frameworks to prevent major accident hazards involving chemicals. However, the huge number of chemicals makes it almost impossible to identify and characterise all the chemicals. To manage this problem, the use of indicative criteria that have adopted the GHS (Globally Harmonised System of Classification and Labelling of Chemicals) can serve to ensure safety in the handling of chemicals and to prevent major accidents. The indicative criteria are used to group chemicals with the same hazards, which are then assigned threshold quantities (TQ) to assess potential chemical risks. Countries like those in the EU, Singapore, China and Australia have adopted indicative criteria associated with GHS into their respective regulations. However, these regulations are not the same. Thus, by learning about practices adopted by these countries, and also taking into account the GHS implementation, this study proposes adopting indicative criteria and relevant TQs to prevent major accidents. We hope that the proposed indicative criteria will be useful, particularly for developing countries that would like to establish or amend their national legislation to prevent major accidents involving chemicals, because besides lacking information about previous accidents, they may also lack a comprehensive chemical database and experts/resource persons.

- **Keywords:** Major accident hazards; Technological disaster; Indicative criteria; GHS; Threshold quantities; Chemical safety

Yunlu Ma, Jianqin Zheng, Yongtu Liang, Jiří Jaromír Klemeš, Jian Du, Qi Liao, Hongfang Lu, Bohong Wang. *Deeppipe: Theory-guided neural network method for predicting burst pressure of corroded pipelines*. Pages 595-609.

Crude oil and natural gas are the primary energy sources, mainly transported by pipelines. Pipeline safety has to be seriously considered to ensure the continuous and stable transportation of these two types of energy sources. The burst pressure is an important indicator of pipeline safety. Accurate prediction of the burst pressure is of great significance to the design, construction, daily operation, and maintenance of the pipeline. This paper proposes a theory-guided neural network model-based method to predict burst pressure prediction of corroded pipelines, which can incorporate physical principles into the deep learning framework. First, higher-order features with physical meaning are constructed and coupled with the original features to form a new feature space. Then the traditional burst pressure prediction formula Pipeline Corrosion Criterion (PCORRC) is integrated into the model to make full use of the prior knowledge contained in the empirical formula. The designed loss function enables the network to have different weights for different samples and focuses on learning the PCORRC formula to predict samples with large deviations. Finally, the model was verified using a public dataset based on experiments and finite element simulations. The results show that the theory-guided neural network model proposed in this paper has the highest accuracy compared with other models. The correlation coefficient is 0.9945, the root mean square error is 0.562, and the mean absolute percentage error is 2.65%. Further tests have shown that the model is very robust and has good adaptability to different data. This work presented that integrating domain knowledge into the traditional neural network

model can effectively improve the performance of burst pressure prediction of the corroded pipeline.

- **Keywords:** Oil and gas; Corroded pipeline; Burst pressure prediction; Neural network; Theory-guided

Ruming Pan, Gérald Debenest, Marco A. B. Zanoni. A robust two-dimensional model for the pyrolysis of plastic waste driven by self-sustaining smoldering. Pages 610-619.

This study established a robust two-dimensional (2D) numerical model for plastic waste (PW) pyrolysis driven by self-sustaining smoldering. The smoldering-driven pyrolysis reactor consists of a smoldering chamber filled with char and sand and a pyrolysis chamber with a porous-matrix bed and PW particles. The PW could be melted and decomposed into value-added volatiles driven by the stable char smoldering heat. The findings revealed that the pyrolysis duration and product distribution could be regulated by the char concentration and Darcy air velocity. Higher PW contents shortened the volatiles' residence time in the pyrolysis chamber and controlled the pyrolysis product yields. The increased PW content could enhance the PW processing capacity potentially resulting in the recovery of more liquid and gaseous fuels. Moreover, the reactor's geometry significantly affected the pyrolysis chamber's temperature distribution and the PW processing capacity.

- **Keywords:** Plastic waste; Pyrolysis; Self-sustaining smoldering; Mathematical model

Oscar de Almeida Neuwald, Márcia Borghetti, Daniele Perondi, Éverton Hillig, Marcelo Godinho. *Steam catalytic gasification of elephant grass pellets*. Pages 620-630.

There is a worldwide consensus on the need to replace fossil energy sources with renewable ones. Biomass is a promising alternative for replacing the use of fossil fuels. In addition, biomass contributes to the reduction of greenhouse gas emissions, since when subjected to a thermal process, it releases carbon dioxide consumed by its photosynthesis, as is the case of the elephant grass. This biomass can be used as an energy source; nevertheless, its low density makes conversion processes difficult (especially in the feeding step). To solve this problem, its densification in the form of pellets can be applied. The main processes for obtaining energy from biomass are the thermochemical processes: pyrolysis, combustion, and gasification. Gasification has high energy efficiency, being a promising alternative for energy generation. The gasification process can be improved through the use of catalysts, in order to increase the yield in the production of syngas (H2 + CO). The alkali and alkaline earth metals (AAEM) can be present in the biomass, or be added to the gasification process, acting in the tar cracking for greater efficiency in the gasification reaction. Potassium (K) is an alkali metal present in biomass, which has a catalytic role in the gasification process, especially when steam is used as gasification agent. Its concentration in biomass can be modified according to the fertilization during the planting of the biomass. Another catalyst for the gasification process is iron (Fe), however this metal is present in low concentrations in the biomass itself and must be incorporated into it before its gasification. The use of iron as a catalyst becomes interesting due to its low toxicity and cost, having the ability to crack tar molecules, hence increasing the gasification yield. Based on this, the effect of potassium and iron as catalysts in the steam gasification process of elephant grass pellets was investigated in this work.

- **Keywords:** Gasification; Biomass; Elephant grass; Catalysts and pellets

Ali Allahyarzadeh-Bidgoli, Mehdi Mehrpooya, Jurandir Itizo Yanagihara. *Geometric optimization of thermo-hydraulic performance of multistream plate fin heat exchangers in two-stage condensation cycle: Thermodynamic and operating cost analyses*. Pages 631-648.

LNG is an energy carrier with growing importance, but LNG cryogenic cycles are energy-intensive. Because the thermo-hydraulic performance of heat exchangers affects the operation and energy consumption of a compressor. The optimization of heat exchangers is key to improving the energy efficiency of a cryogenic plant. In this work, the screening analysis and optimization procedures are performed for a two-stage condensation plant to enhance the Coefficient of Performance (COP) as the operating performance criterion. Five geometric design categories of applied fins, such as fin type, fin height, fin thickness, fin frequency, and the number of layers of MPFHEs (Multistream Plate Fin Heat Exchanger) are selected as input parameters for the optimization process. Then, a thermodynamic analysis including the second law analysis and capital and operating costs assessment are carried out to show the improvements of applied optimization in the mentioned objectives. The results of the optimization procedure have indicated a considerable improvement in the COP of up to 13.7% and significant mitigation in total power consumption of up to 11.8 MW. Furthermore, the optimal configuration of heat exchangers presents an increase in exergy efficiency of up to 4.1%, a saving in exergy destruction of 10.2 MW and up to 8.6 M USD/year in the operating cost when compared with conventional cases.

- **Keywords:** Thermodynamic and cost analyses; Thermo-hydraulic performance; Optimization; Condensation stage; MPFHE

Cheng Ji, Fangyuan Ma, Jingde Wang, Wei Sun, Xuebing Zhu. *Statistical method based on dissimilarity of variable correlations for multimode chemical process monitoring with transitions*. Pages 649-662.

Chemical industrial processes are always accompanied by multiple operating conditions, which brings great challenges for multivariate statistical process monitoring methods to extract general characteristics from multimode data, especially for time-varying characteristics in transitions between two modes. In this work, a novel statistical process monitoring method based on the dissimilarity of process variable correlation (DISS-PVC) is proposed. The proposed method aims to monitor multiple stable modes and between-mode transitions simultaneously with no prior knowledge of the number of operating modes. Unlike traditional methods oriented to monitoring process variables, the proposed method is applied to monitor the correlation of process variables based on the idea that variable correlation should always conform to a certain process internal mechanism, no matter in which stable or transition mode. Mutual information is first employed to quantitate variable correlation with a moving-window approach. Cosine similarity between eigenvalues of mutual information matrices is selected as a dissimilarity index to evaluate the difference in variable correlation between two data sets and perform fault detection. The effectiveness of the proposed method is verified on the benchmark Tennessee Eastman (TE) process and an industrial continuous catalytic reforming heat exchange unit.

- **Keywords:** Multimode process monitoring; Feature extraction; Process safety; Mutual information; TE process; Industrial application

Huijuan Sun, Najiaowa Yu, Yang Liu. *Importance of low-abundance microbial species in response to disturbances in wastewater bioreactors*. Pages 663-671.

This study demonstrates the importance of low-abundance species in maintaining biosystem stability in response to a changing reactor operation condition. Initiation and termination of effluent recirculation were applied as the operational disturbance factors in two upflow anaerobic sludge blanket (UASB) reactors treating high-strength wastewater, respectively. The microbial growth rates during the community evolution were calculated based on the non-steady-state mass balance model. Community evolution studies showed that directly following the initiation/termination of effluent recirculation, the microbial communities reached the highest diversity. The net growth rates of individual microbes during community evolution illustrated that low-abundance species played a critical role in response to the disturbance induced by initiating or discontinuing effluent recirculation. This study highlights the importance of the response of low-abundance species in maintaining biosystem stability when a disturbance is applied to a wastewater bioreactor.

- **Keywords:** Wastewater bioreactor; Disturbance; Effluent recirculation; Low-abundance microbial species; Microbial net growth rate

Huichang Niu, Caixing Chen, Yanhui Liu, Lei Li, Zhao Li, Dan Ji, Xinyan Huang. *Mitigating thermal runaway propagation of NCM 811 prismatic batteries via hollow glass microspheres plates*. Pages 672-683.

The propagation of thermal runaway in Lithium-ion battery modules can escalate fire hazards and damage in energy storage systems. More effective strategies are needed to ensure the safe application of high-energy lithium-ion batteries and alleviate the thermal runaway propagation. This work explores the use of ultra-light plates based on hollow glass microspheres (HGM) as firewalls in the large-format battery module. A systematic experimental study is conducted using the prismatic battery with LiNi0.8Co0.1Mn0.1O2 (NCM 811) cathode and HGM firewalls with different thicknesses. Performance tests suggest that the composite plate with 60 wt% HGM, 25 wt% curing agent, and 15 wt% flame retardant is most effective in mitigating thermal runaway propagation. Without firewalls, the thermal runaway propagation rate increases from 0.43 cell/min to 0.85 cell/min as the SOC level increases from 25% to 100%. Inserting HGM plates can effectively slow down thermal runaway propagation, where the 3-mm HGM plates can successfully block the thermal runaway. A simplified heat transfer model is also proposed to explain the performance of the firewall in inhibiting thermal runaway and help to optimize the safety design for battery modules. This work provides important insights into the thermal runaway risks and safety measures of large battery systems.

- **Keywords:** Battery safety; Composite plate firewall; Fire protection; Thermal insulation plate; Propagation rate

Xuanze He, Chunpeng Zhao, Zhenwen Hu, Francesco Restuccia, Franz Richter, Qingsong Wang, Guillermo Rein. *Heat transfer effects on accelerating rate calorimetry of the thermal runaway of Lithium-ion batteries*. Pages 684-693.

The thermal runaway of Lithium-ion batteries (LIBs) is a fire hazard. The Accelerating Rate Calorimetry (ARC) device is commonly used to investigate thermal runaway parameters of LIBs by assuming adiabatic conditions. However, this assumption ignores internal heat transfer within the cell and external heat transfer at the cell surface. In this work, we conducted ARC experiments using prismatic LiCoO2 cells of 50 mm in side to study the effect of heat transfer limitations. Results show that the external temperature

difference between this cell surface and ARC walls varies between 0 and 1.5 ℃ before thermal runaway and increases from 10 to 130 ℃ while thermal runaway occurs. Ignoring external heat transfer causes the heat of reaction of the cell to be underestimated by 12%. To study the internal heat transfer, two models are developed and show that heat transfer causes an internal temperature difference that causes an error of kinetics estimation, and the error grows with cell size. Ignoring heat transfer leads to errors on the thermal runaway parameters quantified by ARC, and these errors could propagate to battery safety design and predictions. This study contributes to designing better ARC experiments and a better understanding of battery safety.

- **Keywords:** Ignition; Fire; Safety; Energy Storage; Calorimetry

Ganjar Samudro, Tsuyoshi Imai, Alissara Reungsang. *Determination of optimum retention time in an air–cathode single-chamber microbial fuel cell batch-mode reactor by comparing different substrate types and concentrations*. Pages 694-705.

The disadvantages of the air–cathode single-chamber microbial fuel cell (AC-SCMFC) performance can be caused by numerous factors, and retention time (RT) is one such factor. It is difficult to conclude the ideal RT run for the specific tests under the same conditions. To determine the optimum RT for various types of microbial fuel cell (MFC), an AC-SCMFC batch-mode reactor was carried out by comparing different types and concentrations of substrates based on the main parameters of organic removal and power generation. The AC-SCMFC reactor was designed for the effective working volume of 500 mL and operated for 52 d in batch mode with factors being significantly correlated with the performance of the MFC reactor, which were two different substrates, sucrose and acetate, and three different chemical oxygen demand (COD) levels of 400; 1000, and 2500 mg/L (low, medium, and high, respectively) equipped with two graphene nanoplatelets (GNPs)-based electrodes connected to 100 Ω resistance and plugged onto a data logger. The results of this study indicated a significant pattern at the medium level, at which the optimum RT of sucrose was achieved at 24 h and that of acetate at 48 h. In comparison, the performances pattern at low and high levels of both substrates was insignificant to determine the optimum RT. For further application, the recommended RT for both substrates at any concentration is 24 h due to high overall performance, and the optimum RT established in this study could be applied to all types of MFC research, particularly in oxidizable or biodegradable organic ranges, which ensures high performance.

- **Keywords:** Air-cathode single-chamber microbial fuel cell; Batch-mode reactor; Retention time; Substrate type; Substrate concentration

Mishal Alsehli, Fadl A. Essa, Z.M. Omara, Mahmoud M. Othman, Ammar H. Elsheikh, Mamdooh Alwetaishi, Saleh Alghamdi, B. Saleh. *Improving the performance of a hybrid solar desalination system under various operating conditions*. Pages 706-720.

The issue of freshwater shortage is a general problem that touches almost all human beings, and everyone is trying to find creative and practical solutions to try to overcome this problem. In this paper, the proposed desalination system consists of a modified solar still (MSS), parabolic trough solar collector (PTSC), separation unit (SU), and two external condensers (EC). The idea of this proposed device is that the PTSC was utilized to heat the saline feed water to a temperature from which steam can be extracted, and then a separation is made for this steam from the remaining water that has risen in temperature and has not been evaporated to be used as feed water for MSS. Also, MSS has been modified by making all its walls (except for the back wall of the distiller) of glass to obtain a greater amount of absorbed solar radiation. Besides, a double glass

cover for MSS was used instead of the single glass sheet to prevent the heat loss to the atmosphere through the glass cover. The double glass cover is two sheets of glass between which there is a slight vacuum pressure. Regarding the experimental tests conducted through July 2021, the main conclusions of this work can be pointed. It was revealed that at 12:00, the maximum water temperature of PTSC was 55 °C at 20 L/hr (0.33 L/min), where the solar radiation was 1050 W/m². Besides, the effectiveness of PTSC was 60%, and the total accumulated productivity of PTSC was 83 L/daytime (daytime = 9 hrs). Moreover, the total accumulated productivities of conventional solar still (CSS) and MSS with double glass cover were 3330 and 2325 mL/m².daytime, respectively. Therefore, the productivity of MSS with double glass cover was smaller than that of the CSS by about 30%. In addition, the total accumulated freshwater distillate of CSS and MSS with double glass and condenser was 3370 mL/m².daytime and 6150 mL/m².daytime, respectively. As a consequence, the productivity of MSS with double glass and condenser was more than that of CSS by around 82.50%. In addition, the thermal and exergy efficiencies were 31% and 2.54%, respectively for CSS and 47.5% and 3.95%, respectively for MSS with double glass and condenser. Besides, the total productivity of the hybrid system (PTSC and MSS together) was reported as 91.0 L/daytime. Also, the cost of distilled water of proposed hybrid system is 0.008 $/L, and payback period of costs on proposed system is three months. Moreover, the environmental parameters of EPF, φCO2, and Z' for MSS are slightly more than the double of that for CSS.

- **Keywords:** Parabolic trough solar collector; Evacuated tube; Condenser; Separation unit; Solar still; Double glass cover

Marisa Raketh, Prawit Kongjan, Khaliyah Sani, Eric Trably, Benjamas Cheirsilp, Rattana Jariyaboon. *Biodegradation efficiencies and economic feasibility of single-stage and two-stage anaerobic digestion of desulfated Skim Latex Serum (SLS) by using rubber wood ash*. Pages 721-732.

The efficiencies of single-stage anaerobic digestion (SSAD) and two-stage anaerobic digestion (TSAD) of desulfated skim latex serum (DSLS) using various rubber wood ash (RWA) loadings were investigated in this study. The experiments on batch processes showed that DSLS gave a higher yield (6–21%) than raw SLS in both SSAD and TSAD. The highest H2 and CH4 yields of 90.64 and 294.53 mL/g-CODadded were achieved with DSLS using RWA loading of 5 g/L (DSLS5) and 10 g/L (DSLS10), respectively in TSAD (thermophilic and mesophilic conditions, respectively). The maximum 305.09 mL/g-CODadded CH4 yield in SSAD was observed for DSLS10. Total energy recovery in TSAD was 5% higher than that in SSAD. However, the cost assessment on continuous AD using kinetics and yield from the batch experiments suggests longer payback time for TSAD (4.36 years) than for SSAD (2.52 years). TSAD is not economically attractive with DSLS10 due to the large total volume of digesters required. This study revealed that RWA can remove sulfate from SLS to enhance biogas production and reduces H2S in the biogas, while TSAD of DSLS was not attractive compared to the conventional SSAD like for some other substrates reported in the literature.

- **Keywords:** Skim Latex Serum; Two-stage anaerobic digestion; Bio-hydrogen; Bio-methane; Cost assessment

Junyuan Guo, Jianying Jiang, Yihua Chen, Xiaoying Wen, Wenjing Chen, Yifan Wang, Lin Su, Jing Cao. *Synthesis of nZVI-BC composite for persulfate activation to degrade pyrene: Performance, correlative mechanisms and degradation pathways*. Pages 733-745.

In order to achieve efficient adsorptive and oxidative removal of pyrene, a persulfate oxidation system with composite nZVI-BC prepared by loading nano-zero-valent iron on coconut shell biochar as an activator was established and applied. The results of adsorption experiments showed that at pH 3, when the dosages of BC, nZVI and nZVI-BC were all 1.5 g/L, the removal efficiency of pyrene reached 64.9%, 19.0%, and 61.2%, respectively after 120 min of adsorption. The best performance of nZVI-BC-persulfate system was achieved at pH 3, nZVI-BC 1.2 g/L and persulfate concentration 6 mM, and after 60 min of degradation, the removal efficiency of pyrene reached 99.4%. The pre-adsorption process was a promoting-step for pyrene degradation. The conversion of nZVI to Fe2+ and Fe3+ played an important role in the activation of persulfate to produce SO4•− and •OH, both of which were responsible for non-selectively oxidization pyrene. The support of BC could improve the dispersibility and activity of nZVI and improve of the above conversion. The intermediates with relatively lower toxicity were identified during pyrene degradation, and they were successively oxidized into CO2 and H2O finally. In summary, nZVI-BC can be a promising catalyst for persulfate activation to degrade PAHs in wastewater.

- **Keywords:** Pyrene; Biochar; Zero-valent iron; Adsorption; Degradation

Xue Deng, Run Huang, Xiaodong Lv, Jingpiao Yang, Jing Yang. *Separation and recovery of metallic zinc and iron concentrate from blast furnace dust by vacuum carbothermal reduction*. Pages 746-751.

Theoretical calculations and experimental studies were used to investigate a process involving the evaporation, condensation, and separation of blast furnace dust with vacuum carbothermal reduction. The theoretical calculations revealed that the removal rate of metallic zinc from blast furnace dust by vacuum carbothermal reduction was> 99.6%, with a 800–900 °C reduction temperature range. The experimental results showed a 97.8% removal rate of metallic zinc in the reduced sample. The phase transformations of iron and zinc during the reduction process were ZnFe2O4 → Fe2O3 → Fe3O4 → FeO and ZnFe2O4 → ZnO → Zn(g), respectively. Metallic zinc in ZnFe2O4 phase was reduced, condensed, and collected after escaping in the gas form. These results demonstrated the feasibility of a novel process for recovering metallic zinc and high-grade iron-bearing raw materials from blast furnace dust.

- **Keywords:** Metallic zinc; Vacuum carbothermal reduction; Evaporation; Condensation separation; Waste management

Jishuo Li, Xiwen Yao, Ji Ge, Yue Yu, Dexin Yang, Shoukun Chen, Kaili Xu, Liyan Geng. *Investigation on the pyrolysis process, products characteristics and BP neural network modelling of pine sawdust, cattle dung, kidney bean stalk and bamboo*. Pages 752-764.

To realize resource utilization of waste and alleviate associated environmental pollution, the pyrolysis behaviour of pine sawdust (PS), cattle dung (CD), kidney bean stalk (KS) and bamboo (BA) was investigated. The mass loss, gaseous product evolution and kinetic parameters of these four materials during pyrolysis were analysed via TG-MS. According to the TG-MS results, a back propagation (BP) neural network model was developed for the mass loss prediction of different biomass pyrolysis. More importantly, FTIR and SEM-EDX were used to analyse the characteristics of bio-oil and biochar to facilitate further utilization of these pyrolysis products. The results indicated that PS exhibited the highest

mass loss (87.25%) during pyrolysis at 800 °C, and the higher D value (1.23E-05) indicated that PS was more easily decomposed than other materials. In terms of gaseous products, PS produced more H2, C2H6, C3H8 and CO2 than did the other materials during pyrolysis, while BA produced more CH4 and H2O. In addition, the content of phenols or aromatic compounds in PS bio-oil was the highest, and the surface pores in the obtained PS biochar were uniform and regular, which verified that PS achieved a higher utilization value than that of the other materials considered. Finally, the established BP neural network models realized a satisfactory mass loss prediction performance with increasing temperature.

- **Keywords:** Pyrolysis behaviour; TG-MS; Bio-oil; Biochar; BP neural network model

Emilie Gout, Mathias Monnot, Olivier Boutin, Pierre Vanloot, Magalie Claeys-Bruno, Philippe Moulin. *Assessment and optimization of wet air oxidation for treatment of landfill leachate concentrated with reverse osmosis*. Pages 765-774.

Sanitary landfilling is one of the most common ways to eliminate solid municipal/urban wastes. Despite many advantages, this method leads to the generation of contaminated leachates that remains an unavoidable consequence of the waste disposal. Membrane technologies, such as reverse osmosis, are frequently used for leachate treatment as they generate good quality permeate with a high recovery rate. However, their primary drawbacks are fouling, eliminated by chemical wash, and the production of highly polluted concentrates. This paper aims to assess and optimize the use of wet air oxidation to treat reverse osmosis concentrates in terms of bio-refractory organic pollutants removal. Wet air oxidation was performed at elevated pressure and temperature using experimental design methodology with a 70% oxygen excess for 6 h in a stirred batch reactor. The effect of operating conditions was investigated with an experimental design where 3 factors (two quantitative ones: pressure and temperature and a qualitative one: seasonality of the effluent) have been considered. The chemical oxygen demand and the total organic carbon removals increased with the increase of temperature (from 200 °C to 300 °C) and no effect of the pressure was observed within the range 18 – 21 MPa. Wet air oxidation could achieve up to 99% removals for chemical oxygen demand and total organic carbon for the seasonality of October. Experiments also showed that increasing the initial pollutant concentration increased initial kinetic rates. Finally, models were established to calculate and predict pollution removal rate and its kinetic, in the domain of study.

- **Keywords:** Hybrid process; Landfill leachates; Process intensification; Reverse osmosis; Wet air oxidation; Design of experiments

Chris Agida Uko, Jimoh Oladejo Tijani, Saka Ambali Abdulkareem, Saheed Mustapha, Titus Chinedu Egbosiuba, Edison Muzenda. *Adsorptive properties of MgO/WO3 nanoadsorbent for selected heavy metals removal from indigenous dyeing wastewater*. Pages 775-794.

The magnesium oxide/tungsten trioxide (MgO/WO3) nanocomposites were prepared at different mixing ratios using a combination of green and wet impregnation methods and subsequently utilized as nanoadsorbent for the removal of selected heavy metals from Indigenous dyeing wastewater. The synthesized nanomaterials were characterized using High-resolution electron microscopy (HRSEM), High-resolution transmission electron microscopy (HRTEM), Energy Dispersive Spectroscopy (EDS), Selective Area Diffraction (SAED), X-ray diffraction (XRD) and Brunauer Emmett-Teller (BET) N2 Adsorption-desorption method. HRSEM/HRTEM analysis demonstrated the formation of a distinct spherical shape irrespective of the mixing ratio of MgO on WO3 nanoparticles. XRD

analysis confirmed the existence of a monoclinic phase and face centred cubic phase for WO3 and MgO nanoparticles and strong interaction between the nanoparticles leading to the formation of magnesium tungstate (MgWO4). The BET analysis revealed a higher surface area (104.2 m2/g) for mesoporous MgO/WO3 nanocomposite with a mixing ratio (4:1) than WO3 alone with a surface area (22.5 m2/g). The maximum removal efficiency of Cu(II) (98.1%), Fe(II) (100%) and Cr(VI) (100%) was achieved at an optimum contact time of 12, 12 and 14 min respectively. The adsorption data evaluated using Langmuir, Freundlich and Temkin models showed that experimental data best fitted the Langmuir model while the fitness of adsorption data to different kinetic models followed pseudo-second-order. The adsorption of the selected metal ion using MgO/WO3 nanoadsorbent was based on electrostatic attraction, ion exchange, and pore diffusion mechanism. The thermodynamic study demonstrated the endothermic and spontaneous nature of the metal sorption process. MgO/WO3 nanoadsorbent with a mixing ratio (4:1) exhibited greater adsorption efficiency than other nanoadsorbents and has excellent regeneration potentials after 5 cycles.

- **Keywords:** Tungsten trioxide; Magnesium oxide; Indigenous Dyeing Wastewater; Heavy metals; Adsorption technology

Venkata Siva Naga Sai Goli, Prithvendra Singh, Devendra Narain Singh, Love Kush Tak. *Investigations on characteristics of landfill-mined-soil-like-fractions and their dependency on organic matter*. Pages 795-812.

Landfill mining, LFM, is considered to be one of the alternatives to overcome adverse effects of unscientifically created landfills/dumpsites, UCLDs, and engineered landfills, ELFs. However, the feasibility of various pathways for the valorization of its yield, designated as the landfill mined residues, LMRs, for sustainable development is still being debated mainly due to not in-place schemes for comprehensive characterization of the landfill-mined-soil-like-fractions, LFMSF, which is a major component of LMRs. Due to this lacuna, proper guidelines, and strategies for utilization of the LFMSF as a manmade resource could also not be developed so far. Another constraint in this context is that the physicochemical characteristics of LFMSF have been attributed to its age, which is difficult to obtain (if not impossible), due to lack of know-how about the method of disposal, turning, and leveling of MSW, and variation in the decomposition pattern between UCLDs and ELFs. With an intention to address these issues, a comprehensive characterization of LFMSF obtained from some of the UCLDs/ELFs in India was conducted by considering their physical, chemical, mineralogical, and thermal characteristics. Based on the experimentally generated data and its statistical analysis, it has been demonstrated that the characteristics of the LFMSF are primarily influenced by its OM. Subsequently, easy to employ relationships between the OM and the characteristics of LFMSF have been developed. It is believed that these relationships will be very much useful for a quick estimation of the LFMSF characteristics that would be very handy for defining its appropriate applications to fulfill sustainable development goals.

- **Keywords:** Landfill mining; Landfill-mined-soil-like-fractions; Organic matter; Landfill mined residues; Unscientifically created landfills/dumpsites; Engineered landfills; Sustainable development

Sunghyun Cho, Youngjin Kim, Minsu Kim, Hyungtae Cho, Il Moon, Junghwan Kim. *Multi-objective optimization of an explosive waste incineration process considering nitrogen oxides emission and process cost by using artificial neural network surrogate models*. Pages 813-824.

Fluidized bed incinerators are more efficient and safe for treating explosive waste than previous methods because they can emit nitrogen oxide (NOx) concentrations below the standard value (90 ppm). However, a limitation is that they have only focused on

optimizing the operating conditions to minimize NOx emission concentrations till now. In this situation, it is crucial to balance NOx and process costs. Therefore, this study designed an explosive waste incineration process and performed multi-objective optimization. An artificial neural network surrogate modeling method is vital to reduce optimization time. Therefore, surrogate models with 95% and 99% accuracies were obtained, reducing the calculation time by 90%. Furthermore, an index combining NOx emission concentrations and process costs was proposed to obtain an optimal balanced operating condition of the process. By optimizing the process index, a new operating condition was obtained that could reduce 20% of the process costs while maintaining NOx emission concentrations within the standard limit. The proposed operating condition and data, such as from sensitivity analysis, would provide a valuable guideline for operating the abovementioned process associated with NOx emission standards.

- **Keywords:** Explosive waste incineration process; Artificial neural network surrogate model; Multi-objective optimization; Nitrogen oxide emissions; Process cost; Fluidized bed

Li Jia, Shoujian Peng, Jiang Xu, Fazhi Yan, Jieren Chen, Bin Wu, Yuexia Chen. *On the evolution mechanism of permeability during gas drainage: Insights from deformation field, gas pressure field and temperature field*. Pages 825-836.

Permeability is an important factor affecting efficient gas drainage, ensuring coal mine process safety, ecological environment protection and clean energy capture. We develop a gas drainage physical simulation device with multi-physical coupling to study the dynamic response mechanism of permeability during gas drainage and explore the basic relationship between the interaction between boreholes and permeability during parallel borehole drainage. By installing 48 pressure sensors, 14 temperature sensors, and 9 displacement sensors in a test box, gas drainage tests of parallel boreholes with spacings of 250, 504, and 784 mm were carried out. The results show that during gas drainage in parallel boreholes, the dynamic evolution law of permeability in different spatial positions of the coal reservoir has apparent differences. The permeability near the borehole area exhibits a fast decline rate and a large recovery amplitude, and vice versa. The gas pressure, coal deformation, and coal temperature influence the periodical permeability evolution. In the early stage of drainage, gas pressure and coal temperature play a leading role in reducing permeability. In the middle and late stages, coal deformation slowly increases permeability. When the borehole spacing was 250 mm, the permeability decay rate and rebound rate were high with interaction between the boreholes; a drainage superposition area makes the permeability spatial variation difference between the boreholes significant. A correlation is observed between borehole spacing, gas migration rate, and permeability. The study is expected to have a substantial guiding significance for efficient gas drainage, decreasing greenhouse gas emissions, and improving coal mine process safety.

- **Keywords:** Gas drainage; Permeability; Multiple physical field parameters; Borehole space interaction; Parallel boreholes

Jinju Hou, Xiaotong Zhang, Shudong Zhang, Wenjin Hu, Zhiting Kang, Guanwen Yi, Yu Zhou, Yunuo Huang, Qiuzhuo Zhang. *Improvement of bioethanol production using a new fermentation system: The process analysis and micro-mechanisms study*. Pages 837-845.

Rice straw based bioethanol is a clean alternative energy source to alleviate the energy crisis and greenhouse gases emission. However, the efficient alkali pretreatment of rice straw for bioethanol production will generate several fermentation inhibitors, such as ferulic acid, which could inhibit bioethanol fermentation. Therefore, an adsorbent called

Air Environment-Prepared Adsorbent at 250 ℃ (AEPA250) was prepared using the enzymatically hydrolyzed residue of rice straw to detoxify ferulic acid in this study for enhancing the subsequent bioethanol production. Analysis of the mass balance showed that ferulic acid detoxification by AEPA250 had a high removal efficiency of 94.393% with a low glucose and xylose loss of 2.532% and 8.219%, respectively. A higher 277.551 mg/L bioethanol concentration and 76.005% glucose consumption rate in the SSBP system were obtained compared to non-detoxified sample. Furthermore, proteomics analysis indicated that certain metabolic pathways of TCA cycle and ribosome pathway as well as various coded proteins of ACO1, MRP2, RPL24B, MRPL33, RPL32, RPL39, RPS17B, RPS19A, RPS26A and ATP5 contributed to ferulic acid detoxification in the SSBP system. The findings of this study may help develop efficient pretreatment methods, detoxification strategies and engineering yeast strains for improving bioethanol production in the future.

- **Keywords:** Bioethanol production; Ferulic acid detoxification; Mass balance; Adsorbent; Proteomics

Yueyue Shi, Yongqi Liu, Yuqi Zhou, Peng Sun, Mingming Mao, Yuqiu Zhang. *Study on dynamic heat extraction characteristics of heat exchanger tube embedded in thermal flow reverse reactor for heat recovery*. Pages 846-858.

In industry, the thermal flow reverse reactor (TFRR) is considered to be an effective means to reduce ventilation air methane (VAM) from fossil fuel operations. The purpose of VAM combustion is either to reduce the emission of greenhouse gas, to recover energy, or both these subjects. The heat exchanger tubes have been embedded on both sides of high-temperature zone of the regenerative oxidizer for heat recovery in this study to improve economy. The mathematical model is established, as well as the effects of inlet methane concentration and air flow rate on dynamic heat extraction characteristics of heat exchanger tubes under periodic conditions are investigated. The results show that sustainable and stable heat recovery can be achieved when the concentration is greater than 0.6 vol.% and the air flow rate is less than 596 m3/h. Heat extraction mainly depends on downstream heat exchange tubes. The asymmetry of heat transfer process between upstream and downstream heat exchanger tubes is analyzed. It is worth noting that the asymmetry is improved at high inlet methane concentration and low air flow rate. The heat recovery efficiency by the bilateral heat exchanger tubes is 61.72% at most, which provides a reliable theoretical basis for the heat extraction mechanism of the heat exchanger embedded in TFRR.

- **Keywords:** Heat recovery; Dynamic heat extraction characteristic; Heat exchanger tubes; Periodic conditions; Regenerative oxidizers

Dong Zhang, Hanhan Li, Xiao-San Luo, Weijie Huang, Yuting Pang, Jinshan Yang, Mingwei Tang, Tariq Mehmood, Zhen Zhao. *Toxicity assessment and heavy metal components of inhalable particulate matters (PM2.5 & PM10) during a dust storm invading the city*. Pages 859-866.

Dust storm (DS) represent global air pollution and health issues considering the high morbidity and premature death rate every year. This study explores the characteristics, composition, and variations in inhalable particulate matters (PMs) as well as their corresponding in vitro toxicity to human lung epithelial cells (A549) during DS and normal days (ND) in the downtown (DT) and the north suburban (NS) of Nanjing city, eastern China. Results showed that compared to ND, concentrations of heavy metals (i.e., Cr, Cu, Ni, and Pb) bound in PMs were lower during the DS. Furthermore, the relationship of cytotoxicity with Ni and Pb levels in PMs was significant. However, the

cytotoxicity difference was insignificant between NS and DT. This may be due to the long-range transport of components from natural sources mixed with local pollutants emitted from anthropogenic sources, offsetting the pollution difference between urban and suburban areas. During both periods, PM2.5 toxicity was greater than PM10, while the potential of PM10 to induce proinflammatory cytokines was comparable to PM2.5. Results suggested that inflammation risk will increase significantly during DS due to a substantial increase in ambient air PM10 concentration.

- **Keywords:** Dust storm; Human lung epithelial cell line; Oxidative stress; Inflammation; Cytotoxicity; Heavy metals

Mohammad Hossein Keshavarz, Mohadeseh Rezaei, Seyyed Hesamodin Hosseini. *A simple approach for prediction of Henry's law constant of pesticides, solvents, aromatic hydrocarbons, and persistent pollutants without using complex computer codes and descriptors*. Pages 867-877.

A novel approach is introduced for reliable prediction of Henry's law constant of persistent pollutants, pesticides, aromatic hydrocarbons, and solvents, which have extensive use for the description of the movement of chemical compounds inside and outside aquatic ecosystems. The largest available experimental data of Henry's law constant for 530 heterogeneous chemicals are used to develop and test the novel model. This method needs the molecular structure of the chosen heterogeneous compound that is based on four non-additive factors including the contributions of hydrogen bonding functional groups, polar groups, halogenated compounds, hydrocarbons as well as the number of specific atoms as additive parameters. Internal and external validations are done on the estimated results for 353 and 177 chemicals of training and test sets, respectively. Various statistical parameters containing correlation coefficient (R2), the maximum value of errors (MaxError), mean error (ME), and root mean squared error (RMSE) are also used to confirm the high reliability of the novel correlation as compared with the best existing method, which requires complicated descriptors. The values of training set R2, MaxError, ME, and RMSE for the new/comparative models are 0.9512/0.8622, 1.521/4.417, 0.0000/0.0194, and 0.4632/0.7797, respectively. The same trend the mentioned statistical parameters also exists for the test set, which confirms the new correlation has higher reliability, goodness-of-fit, accuracy, and precision in comparison to the best available method.

- **Keywords:** Henry's law constant; Heterogeneous compound; Molecular structure; Effective structural parameter; Compound's volatility

Qian Lyu, Gui Fu, Yuxin Wang, Jing Li, Meng Han, Feng Peng, Chun Yang. *How accident causation theory can facilitate smart safety management: An application of the 24Model*. Pages 878-890.

Smart safety management (SSM) in organizations is an inevitable trend in a more intelligent era. However, the adoption of safety science theory lags behind the application of intelligent technology in SSM, posing several challenges (functional dispersion, low-quality data, and lack of versatility). Thus, the accident causation theory (ACT) is adopted to address the existing problem. This study develops a conceptual framework for SSM using the 24Model, a popular ACT in China. The main work conducted in this study is summarized as follows: (a) the description of 24Model and its characteristics, as well as an analysis of its feasibility and applicability in SSM; (b) a detailed presentation of the functions, operation principle, and control paths of unsafe acts in the 24Model-based SSM framework; and (c) a discussion of the framework's advantages, limitations in this research, and suggestions for future research. Research shows that the SSM framework based on the ACT can integrate the functions of the current SSM, establish management sustainability, enhance data quality, and ensure the versatility of the industry, which are

the key factors that facilitate SSM. This study can offer a theoretical and practical basis for safety management in the intelligent era and provide implications for the application of the ACT.

- **Keywords:** Smart safety management; Solution design; Accident causation theory; 24Model

Xie Xuecai, Shu Xueming, Fu Gui, Shen Shifei, Jia Qingsong, Hu Jun, Wu Zhirong. *Accident causes data-driven coal and gas outburst accidents prevention: Application of data mining and machine learning in accident path mining and accident case-based deduction*. Pages 891-913.

Analyzing the causes of accidents, excavating accident paths, and applying accident prevention are important tasks in safety management. Focusing on coal and gas outburst accidents, this study examined the primary accident path and conducted applied research on the reasoning of the accident case. First, combined with the obtained accident causes, a coupling analysis of the causes of coal and gas outburst accidents was conducted. Second, using the method of data mining coupled with Apriori algorithm, the coupling relationship between each cause module of the coal and gas outburst accident was obtained, and consequently, a path map of the coal and gas outburst accident was drawn. Third, a Bayesian network model for the causes of coal and gas outburst accidents was established based on the accident path map and the probability of occurrence of each cause. Finally, considering the safety concept element (SC1) as an example, the Bayesian network model was used to conduct a sensitivity analysis of accident causes. Thereafter, considering the coal and gas outburst accident of the Sanjia Coal Mine in Guizhou Province as an example, probabilistic reasoning research on the cause of the accident was conducted. The application results showed that (1) under normal conditions, there are approximately 797,280 accident paths for coal and gas outbursts. Following data mining, 188 main accident paths were found. (2) Sensitivity analysis determined 19 factors that were sensitive to safety concept elements (SC1), of which the three most sensitive factors were (i) resource management system procedures (SM7), (ii) safety policy (SM1), and (iii) safety training system procedure (SM8). 13 paths exhibited a sensitivity ≥0.5%, of which 7 exhibited strong sensitivity. (3) The absolute accuracy rate of accident cause reasoning in the Sanjia Coal Mine in Guizhou Province was 71.43%, while the relative accuracy rate was close to 100%. Thus, it was concluded that: (1) the accident path mining method proposed in this paper is feasible for main accident path mining. (2) The Bayesian network model for the causes of coal and gas outburst accidents established in this study can be practically applied for the sensitivity analysis of accident causes and exhibits high reliability in the probabilistic reasoning of accident causes. The results of this study is expected to aid in the prevention of coal and gas outburst accidents, and provide reference and help for the path mining of other accident causes and the probabilistic reasoning of accident causes.

- **Keywords:** Coal and gas outburst; Accident causes data driven; Accident paths mining; Accident cause sensitivity analysis; Accident case-based deduction; Apriori-Bayesian algorithm

Seunghwan Ahn, Euijin Shim, Yeonsang Kim, Youn-Sang Bae, Hyeonjin Eom. *Air filtration performance enhancement of PTFE foam–coated filters at high temperatures via secondary strongly adhering PTFE nanofiber coatings*. Pages 914-922.

A PTFE nanofiber–coated PG filter (that is, a modified PTFE foam–coated glass fabric filter (PG filter)) is developed with superior particulate matter (PM) collection efficiency under high-temperature conditions. A modified electrospinning solution is used to coat the PTFE foam surface of the PG filter with nanofibers (precursors to PTFE nanofibers); this

electrospinning solution contains poly(ethylene oxide) whose amphipathicity promotes adhesion between the nanofibers and PTFE foam. Consequently, a PTFE NF–coated PG filter shows enhanced adhesion between the PTFE nanofibers and PTFE-foam surface of PG filter. The PM collection efficiency of and pressure drop across the proposed PTFE nanofiber–coated PG filter were investigated at various temperatures; the air filtration performance of filter exceeds that of a conventional PG filter. In particular, the PM1.0 collection efficiency of the PTFE nanofiber–coated PG filter is 1.13 times higher than that of a PG filter at 280 °C.

- **Keywords:** PTFE nanofibers; PTFE foam; Electrospinning; Air filter; Heat resistance; Particulate matter

Zhiyong Shu, Gang Lei, Wenqing Liang, Wenxiao Dai, Fuming Lu, Xiaohong Zheng, Hua Qian. *Experimental investigation of hydrogen dispersion characteristics with liquid helium spills in moist air*. Pages 923-931.

As green energy, Liquid hydrogen promises to be widely used in the future. However, its security issue has become a great concern because liquid hydrogen will quickly form a low-temperature, flammable, and explosive vapor cloud when leaking or spilling occurs. In this work, liquid helium spilling experiments were designed and performed to predict the dispersion characteristics of liquid hydrogen in confined space with controlled and comparable boundary conditions. The concentration cloud and the infrared cloud images near the liquid helium pool were obtained at the same time. Results show that the air humidity has an impact on the vapor cloud temperature change, i.e., every 10% increase in air humidity will lead to a 5 ℃-temperature increase. The presence of high air humidity increases the vapor cloud buoyancy and promotes the cloud's dispersion in the vertical direction. The visible range of the helium vapor cloud is much smaller than the measured combustible concentration range with air humidity of 50–70%. The helium vapor concentration range at different vertical heights and horizontal distances also increases with the air humidity. The experimental data fits the cloud concentration decay curve under different ambient humidity satisfying the exponential function. The work is expected to provide a technical basis for safety studies of liquid hydrogen and liquid helium spilling.

- **Keywords:** Liquid helium; Dispersion characteristics; Safety scope; Air humidity; Experiment

Xinhong Li, Yujiao Zhu, Rouzbeh Abbassi, Guoming Chen. *A probabilistic framework for risk management and emergency decision-making of marine oil spill accidents*. Pages 932-943.

Offshore oil spills may pose a severe threat to marine ecological environment. In this paper, a new methodology based on Bayesian network (BN) and Influence Diagram (ID) is developed for risk management and emergency decision-making of marine oil spill accidents. The methodology integrates risk management before accident and emergency response after accident, which can balance risk and cost, and render an optimal decision-making. Marine oil spill scenarios including root causations, intermediate and consequent events are identified and modeled using BN considering the dependencies and multi-state of incident process nodes. The probabilities of offshore oil spill incident and the resulting ecological disasters are estimated. The prevention and mitigation measures marine oil spill incidents are identified and added to BN for developing Bayesian ID model, in which the cost and utility of implementing each safety measure are considered. Bayesian ID model can estimate the cost and utility of all safety strategies, and the optimal risk management and emergency strategy are determined by balancing the cost and utility. A case study of marine oil spill accident due to subsea oil pipeline leak is used to illustrate

the methodology. It is observed that the methodology can efficiently support the decision-making of oil and gas sector in risk management and emergency response of offshore oil spill accidents.

- **Keywords:** Offshore oil spill accident; Risk management; Decision-making; BN; Bayesian influence diagram

Huifen Yin, Jing Liu, HanLu Shi, Lei Sun, Xiangjuan Yuan, Dongsheng Xia. *Highly efficient catalytic ozonation for oxalic acid mineralization with Ag2CO3 modified g-C3N4: Performance and mechanism*. Pages 944-954.

A series of Ag2CO3 doping g-C3N4 composites labeled as AgCNx-T (x represented the weight content of g-C3N4 and T referred to the hydrothermal temperature) were synthesized by a simple precipitation method. Various techniques such as BET, XRD, FTIR, SEM, and XPS were employed to explore the morphology structure and physicochemical properties of catalysts ascribed to the decoration of Ag2CO3 onto g-C3N4 and the results revealed that the hydrothermal temperature played an important role in the size dimension and crystallinity of Ag2CO3. It was worthy noted, the decorating of Ag2CO3 would provide more active sites on the catalyst surface, strengthen the regeneration and transmission of electrons, improve the utilization of O3, and promote the generation of reactive oxygen species, thus improving the catalytic ozonation performance. Amongst, the AgCN0.4-100 composite had the optimal performance with 99.99% of OA degradation efficiency and 93.19% of OA mineralization. Moreover, the AgCN0.4-100 exhibited satisfactory reusability for multiple consecutive cycles (≥5) with low Ag ion release (<0.3 mg L−1). The reactive species (O2•− and 1O2) were verified to take predominant roles in the reaction through the radical scavenger experiments and ESR spectra. Accordingly, an empirical kinetic model was established to predict OA concentration with the given operational parameters. Finally, the synergistic mechanism of OA degradation in catalytic ozonation system was also proposed, which possessed promising prospect in practical water treatment for environmental applications.

- **Keywords:** G-C3N4; Ag2CO3; Catalytic ozonation; Oxalic acid; Mechanism

Siping Yang, Jing Yang, Jia Tang, Xiaoqin Zhang, Jun Ma, Aiping Zhang. *A comparative study of the degradation of refractory organic matter in MBR effluent from landfill leachate treatment by the microwave-enhanced iron-activated hydrogen peroxide and peroxydisulfate processes*. Pages 955-964.

This study applied two advanced oxidation processes dominated by different reactive oxygen species (ROS), microwave-iron-hydrogen peroxide (Microwave/ZVI/H2O2) and microwave-iron-peroxydisulfate (MW Microwave/ZVI/PDS), to the degradation of refractory organic matter in the membrane bioreactor (MBR) effluent from landfill leachate treatment. The two processes were systematically compared according to their degradation efficiencies and transformation mechanisms toward refractory organic matter in MBR effluent. Controlled experiments and an influential factor analysis showed that the total organic carbon (TOC) removal efficiencies of the Microwave/ZVI/H2O2 and Microwave/ZVI/PDS processes were 74.48% and 64.40%, respectively. After treatment by the two processes, fulvic-like substances with a low molecular weight and high fluorescence frequency, and humic-like substances with a large molecular weight, stable chemical structure, and high aromaticity were substantially degraded. In addition, the Microwave/ZVI/H2O2 process had a better TOC removal efficiency than the Microwave/ZVI/PDS process over a wider pH range (3−11), which was mainly attributed to the different dominant ROS in the two processes. Both Fe3O4 and FeOOH were found in the reacted ZVI of the two processes, and the reaction mechanisms included Fenton-

like reactions and adsorption-precipitation by iron (hydro)oxides, which were promoted by microwave irradiation. This study provided a theoretical reference for the efficient treatment of MBR effluent.

- **Keywords:** Landfill leachate; Microwave irradiation; ZVI; Hydrogen peroxide; Peroxydisulfate; Refractory organic matter

K.G.V.K. De Silva, M.Y. Gunasekera, A.A.P. De Alwis. *Development of a risk informed quantitative decision making framework for major accident hazards installations in Sri Lanka*. Pages 965-977.

This paper proposes a risk informed decision-making framework for siting Major Accident Hazard Installations in Sri Lanka. It is named the "Upper Bound FN curve" method. Generic failure rate data are utilized as country specific data are not available. FN Curves are derived for each process node of a Major Accident Hazard Installation using different failure rate data sets available in literature. The data sets giving the "worst case" FN Curve for each process node is identified. These FN Curves are called the Upper Bound FN Curves. Using these curves, a composite FN Curve is developed which is compared against the country specific risk acceptance criterion line. If the risk is not acceptable, further safety barriers are introduced. Safety distances are then determined using a scaling factor developed in this study called the relative risk reduction factor (RRRF). The RRRF is determined based on the comparative position of the composite FN curve with respect to the criterion line. The proposed methodology was applied in a case study of liquefied propane storage tank. Guidelines for application of the proposed framework, interpretation of the "Upper Bound FN Curve" method and estimation of safety distances are presented.

- **Keywords:** Major accident hazard; Societal risk; Failure rate; FN curve; Safety distance

Kai Zhang, Saifeng Du, Hao Chen, Jingui Wang, Jiaqing Zhang, Yi Guo, Jin Guo. *Effect of hydrogen concentration on the vented explosion of hydrogen-air mixtures in a 5-m-long duct*. Pages 978-986.

A series of vented hydrogen-air explosion experiments were carried out in an end-vented rectangular tube, and the effect of hydrogen concentrations varying from 10% to 50% on the flame evolution and the maximum overpressure inside and outside the duct were investigated. Experimental results reveal that the flame behavior was strongly affected by hydrogen concentration: the flame speed at the vent exit first increased and then decreased as hydrogen concentration was increased; a tulip flame and two bright fireballs were respectively observed within and outside the duct in some tests. Two dominant pressure peaks and two types of oscillations could be distinguished in the internal pressure curves, corresponding to the rupture of the membrane, venting of the burned gas, Helmholtz, and acoustic oscillations, respectively. Under the current experimental conditions, the pressure peak with a low amplitude owing to the rupture of membrane dominated the external pressure–time histories for hydrogen concentrations less than 25%. However, when the hydrogen concentration ranged from 30% to 50%, the pressure peak caused by the second external explosion become dominant. Besides, the influence of the external explosions on the internal pressure peak structures was discussed. As hydrogen concentration was increased, the maximum internal overpressure first increased and then decreased, whereas the maximum external overpressure increased monotonically. In this study, the maximum reduced overpressures calculated by Molkov's best-fit model agreed well with the experimental data for near-stoichiometric and rich hydrogen-air mixtures.

- **Keywords:** Hydrogen safety; Vented hydrogen-air explosion; Overpressure; Flame; External explosion

Hao Sun, Ming Yang, Haiqing Wang. *Resilience-based approach to maintenance asset and operational cost planning*. Pages 987-997.

Reliability-based and risk-based methods for directing maintenance activities play a critical role in ensuring system safety and reducing unnecessary downtime. Those methods focus on preventive maintenance to avoid component failures and are applicable before unexpected disruptions occur. However, when disruptions are unavoidable, more attention should be paid to systems' recovery from unwanted changes. As a remedy of preventive maintenance, improving system restoration capacity of resilience through optimizing the system's maintenance asset and operational cost is an efficient way to help system restore from disruption conditions within an optimal cost. In this paper, a resilience-based approach is proposed to optimize maintenance asset and operational cost. A novel resilience metric is developed and utilized to quantify system resilience under various restoration capacities. The minimal acceptable resilience level (MARL) and maximal acceptable restoration time (MART) are proposed to determine the optimal maintenance cost. The proposed approach is applied to the Chevron Richmond refinery crude unit and its upstream process. The results show that it can help practitioners identify the optimal cost to ensure a system is resilient to respond to uncertain disruptions and provide a dynamic resilience profile to support decision-making.

- **Keywords:** Resilience; Maintenance; Restoration; Process systems; Cost optimization

Fayza Yulia, Agustino Zulys, Bidyut Baran Saha, Takuya Mabuchi, William Gonçalves, Nasruddin. *Bio-metal-organic framework-based cobalt glutamate for CO2/N2 separation: Experimental and multi-objective optimization with a neural network*. Pages 998-1014.

The outstanding properties of metal-organic frameworks (MOFs) have proven that this type of crystalline adsorbent has great potential in CO2 capture applications. Most of the MOF research studies on new functional MOFs are conducted to improve the performance of CO2 gas adsorption. Combined studies of material evaluation and process design on engineering issues in CO2 capture applications in industry are rarely carried out. In this study, the authors attempted to address engineering issues by developing a biometal-organic framework with the bioligand L-glutamic acid that has more practical fabrication cost than petrochemical MOFs. Herein, the demonstration of the prediction and optimization of CO2 adsorption capacity, selectivity, and heat of adsorption using a multiobjective genetic algorithm (MOGA) combined with an artificial neural network (ANN). The success of the Bio-MOF fabrication was evaluated by scanning electron microscopy, N2 adsorption-desorption isotherm analysis, thermal gravimetric analysis, X-ray diffraction, and Fourier transform infrared spectroscopy techniques. Furthermore, volumetric measurements were performed at several temperatures (27, 35 and, 50 °C). The isosteric heat of adsorption was then evaluated by an indirect method with the Clausius-Clapeyron (C-C) and Chakraborty, Saha, and Koyama (CSK) equations. Then, CO2/N2 selectivity was analysed by IAST techniques by regressing the experimental data with the Langmuir-Freundlich isothermal equation. The computational study by ANN and MOGA also gives satisfying results in balancing three requirements criteria. Thus, this study paved the way for the development of low-cost scalable MOF fabrication in industry by applying the optimization and balancing principles of the three objective functions.

- **Keywords:** Adsorption; CO2/N2; Bio-MOF (bio-metal-organic framework); CO2 capture; Cobalt glutamate; Neural network optimization

Mohamad-Javad Mehrani, Faramarz Bagherzadeh, Min Zheng, Przemyslaw Kowal, Dominika Sobotka, Jacek Mąkinia. *Application of a hybrid mechanistic/machine learning model for prediction of nitrous oxide (N2O) production in a nitrifying sequencing batch reactor*. Pages 1015-1024.

Nitrous oxide (N2O) is a key parameter for evaluating the greenhouse gas emissions from wastewater treatment plants. In this study, a new method for predicting liquid N2O production during nitrification was developed based on a mechanistic model and machine learning (ML) algorithm. The mechanistic model was first used for simulation of two 15-day experimental trials in a nitrifying sequencing batch reactor. Then, model predictions (NH4-N, NO2-N, NO3-N, MLSS, MLVSS) along with the recorded online measurements (DO, pH, temperature) were used as input data for the ML models. The data from the experiments at 20 °C and 12 °C, respectively, were used for training and testing of three ML algorithms, including artificial neural network (ANN), gradient boosting machine (GBM), and support vector machine (SVM). The best predictive model was the ANN algorithm and that model was further subjected to the 95% confidence interval analysis for calculation of the true data probability and estimating an error range of the data population. Moreover, Feature Selection (FS) techniques, such as Pearson correlation and Random Forest, were used to identify the most relevant parameters influencing liquid N2O predictions. The results of FS analysis showed that NH4-N, followed by NO2-N had the highest correlation with the liquid N2O production. With the proposed approach, a prompt method was obtained for enhancing prediction of the liquid N2O concentrations for short-term studies with the limited availability of measured data.

- **Keywords:** Prediction accuracy; Mechanistic model; Machine learning; Nitrous oxide; Nitrification; GHG mitigation

Shun-xiang Shi, Chun-chen Nie, Wen-tao Zhou, Xiang-nan Zhu. *Calorific value recycling of low-value metal leaching residues in waste printed circuit boards assisted by debromination*. Pages 1025-1032.

Metals in waste printed circuit boards (WPCBs) are usually recovered by hydrometallurgical processes. The reuse of leached residues, i.e. non-metallic components, has become a new challenge. In this study, the calorific value properties of leached residues with various particle sizes were studied to explore their potential utilization value. In order to realize the clean recovery of calorific value, bromine in resin was debrominated by pyrolysis. The morphology and phase of the leaching residue were analyzed by scanning electron microscope (SEM) and X-ray diffraction (XRD), the results show that the residue is mainly composed of irregular resin particles. Subsequently, thermogravimetric analyzer was adopted to determine the pyrolysis characteristics, the resin particles were debrominated and pyrolyzed in a tubular furnace, the composition and functional groups of the pyrolysis products were analyzed by gas chromatography mass spectrometer (GC-MS) and fourier transform infrared spectroscopy (FT-IR). The results show that the optimal pyrolysis temperature of the residue is 300–400 °C. Both calcium carbonate and calcium hydroxide can achieve effective debromination. Pyrolytic oil, as the main pyrolysis product, is mainly composed of phenols. Finally, the calorific value of pyrolysis products was measured by calorimeter, and the calorific value of pyrolysis oil and pyrolysis residue reached 31.72 MJ/kg and 8.54 MJ/kg. Therefore, leached residues have the potential as a secondary fuel. The ultimate goal is realize the clean and harmless treatment, a comprehensive utilization method of the leach residue of metal components in WPCBs was proposed.

- **Keywords:** Waste printed circuit boards; Clean recovery; Leaching residue; Debromination pyrolysis; Calorific value

Poku Gyasi, Jiandong Wang. *Design of serial alarm systems based on deadbands and delay timers for removing false alarms*. Pages 1033-1041.

Alarm deadbands and delay timers are widely used in practice to remove false alarms. This paper proposes a method to design serial alarm systems that are composed of alarm deadbands serially followed by delay timers. Serial alarm systems are effective for removing false alarms with different types of alarm deviations and alarm durations, while alarm deadbands or delay timers alone are suitable only for one type of false alarms. A minimization problem is formulated to simultaneously design optimal values of the alarm deadband width and delay timer factor, for achieving a desired ratio of false alarms to be remove. Bayesian estimation approach is exploited to resolve a main technical challenge in achieving reliable estimates of joint probabilities of alarm deviations and alarm durations. Existing methods are confined to the isolated design of alarm deadbands or delay timers based on probability density functions of process variables, and are subject to a restrictive assumption that process variables are independent and identically distributed. By contrast, the proposed method is for the joint design of serially-connected alarm deadbands and delay timers; it is based on joint probabilities of alarm deviations and alarm durations, and does not require the restrictive assumption. Numerical and industrial examples are provided to illustrate the proposed method and compare with existing ones.

- **Keywords:** Alarm systems; False alarms; Alarm deadbands; Delay timers; Bayesian estimation

Marco Bellegoni, Claudio Chicchiero, Gabriele Landucci, Chiara Galletti, Maria Vittoria Salvetti. *A UQ based calibration for the CFD modeling of the gas dispersion from an LNG pool*. Pages 1043-1056.

The modeling with Computational Fluid Dynamics (CFD) of gas dispersion from a liquified natural gas (LNG) pool is investigated in detail to better elucidate the sources of uncertainties and the influence of physical phenomena, such as convection and diffusion, just above the pool. Indeed, a better comprehension of these topics can improve gas dispersion analysis and aid the implementation of mitigation measures. However, the literature shows a lack of knowledge on this matter, since the LNG pool inlet conditions have not been precisely analyzed so far. To this purpose, the present work proposes, for the first time in this field, the application of an Uncertainty Quantification (UQ) technique to calibrate the inlet conditions of a CFD model for cloud dispersion from a LNG pool. More specifically, the Burro test series is used to validate numerical simulations based on the solution of Unsteady Reynolds-averaged Navier-Stokes (URANS) equations. As the LNG is released into a water pool, the real LNG pool radius is unknown. Moreover, the gas release is also unknown as it is not equal to the LNG spill rate. The generalized Polynomial Chaos (gPC) expansion is therefore used to estimate these uncertain parameters, by minimizing the errors between CFD and available measurements. The optimization performed on the Lower Flammable Limit (LFL) concentration maps shows how this procedure can give a very good agreement with the experimental observations, extending the accuracy of CFD simulations within risk assessment studies. Besides, this approach highlights how the influence of convection and diffusion on the simulation results strongly depends on the wind conditions. In this manner, the present work can help modelers to better setup CFD simulations with the purpose to aid the decision making in the process safety framework.

- **Keywords:** CFD; RANS simulations; Liquefied natural gas; Gas dispersion; Uncertainty quantification

Sun-A An, Jonghun Lee, Jeonghoo Sim, Cheol-Gyu Park, Jin-San Lee, Hojung Rho, Kwang-Duck Park, Han-Seung Kim, Yun Chul Woo. *Evaluation of the advanced oxidation process integrated with microfiltration for reverse osmosis to treat semiconductor wastewater*. Pages 1057-1066.

This study evaluated the filtration performance and energy consumption of three different reverse osmosis (RO) membranes (ESPA2-LD, RE4040-BE, and TMG10D) for treating semiconductor wastewater. A ceramic membrane combined with ozone for RO pre-treatment and the influence of ozone injection on the filtration and energy consumption efficiency of RO were investigated. A flat-sheet ceramic membrane comprising Al2O3/SiO2-ZrO2 was used to treat real and synthetic semiconductor wastewater as feed water. The deionized water (DI) permeabilities of RO membranes were 144.6, 94.22, and 156.6 LMH/bar, respectively. The microfiltration process that used ozone reduced the permeability of all RO processes, and the total organic carbon (TOC) removal rate decreased when ozone was applied. The application of ozone on power consumption was inconclusive, and its effect was unclear indicating an increase 3.37%, 4.48%, and 11.6% when filtrated with ozone, respectively. TMG10D showed the highest permeability followed by ESPA2-LD and RE4040-BE, for both, the real and synthetic wastewaters. However, ESPA2-LD showed the highest salt and TOC rejection followed by RE4040-BE and TMG10D. TMG10D exhibited the lowest energy consumption per ton of filtered water followed by ESPA2-LD and RE4040-BE. ESPA2-LD was determined to be the most suitable membrane in terms of the water quality stability and energy consumption in RO to treat semiconductor wastewater.

- **Keywords:** Reverse osmosis; Wastewater remediation; Ceramic microfiltration pretreatment; Advanced oxidation; Semiconductor wastewater

Shuang Li, Mengjie You, Dingwei Li, Jiao Liu. *Identifying coal mine safety production risk factors by employing text mining and Bayesian network techniques*. Pages 1067-1081.

Coal industry is a typical high-risk industry with frequent accidents. In an effort to ensure workers' safety and health, and reduce the probability of productivity decrease, it is essential to identify the contributing factors of coal mine safety production risks through certain technical means. Accident cases, as a concentrated display of accident hazard source, are of great value in extracting key risk factors that may induce coal mine disasters. Therefore, this study creatively proposed an effective method combining text mining, association rule mining and Bayesian network to deeply mine and use the massive coal mine safety accident case text data, so as to achieve effective identification of coal mine safety risk factors and explore the mechanism of interaction between risk factors and their importance. The research main included three steps. First, due to the high uncertainty and difference in the way of expression of the coal mine accident report texts, the conventional text mining process cannot effectively identify the risk factors, resulting in the incompleteness and deviation of the risk factors list. This study improved the text mining process, through Chinese word segmentation, keyword extraction, related word mining, semantic analysis, etc. to mine the collected 726 reports, and identify 78 safety risk factors. Then, the Apriori algorithm was used to obtain the extremely frequent itemset of risk factors and 362 strong association rules, and constructed the Bayesian network model on this basis. Finally, six main risk factors of coal mine safety production and their associated-factors were clarified through sensitivity and critical path analysis. The study shows that compared with the risks caused by the environment and equipment, the lack of management, education, and supervision are the root cause of coal mine accidents. This research provides a new way of thinking for effectively extracting using information from unstructured and non-standardized texts, as well as a new perspective for data-driven safety risk factors identification and complex

interaction mechanisms research, having a great significance for coal mine safety risk pre-control management.

- **Keywords:** Risk factor identification; Coal mine safety; Text mining; Bayesian network; Association rule mining

Limei Wang, Yanfei Pan, Yulin Li, Zhuyin Sui, Jisen Li, Xiufeng Xu. *Destructive sorption of NF3 as a novel greenhouse gas over Al2O3 @Mn2O3 sorbents with high surface area*. Pages 1082-1090.

Destructive sorption of NF3 as a novel greenhouse gas on the metal oxides sorbents is an effective way for its destruction. The key issue is to develop an active sorbent for NF3 destruction. Here, AlOOH supported on carbon sphere (CS@AlOOH) was synthesized hydrothermally and calcined to produce Al2O3. Subsequently, the Al2O3 was coated hydrothermally by MnOx at various temperatures and heat-treated to prepare the Al2O3 @Mn2O3 sorbents with core@shell structure for NF3 sorption. The results show that the higher surface area/pore volume and the promotional effect of surface Mn2O3 on the fluorination of Al2O3 substrate led to higher reactivity of Al2O3 @Mn2O3 sorbents than bare Al2O3 in NF3 destruction. For Al2O3 @Mn2O3 sorbents, the coating temperatures of MnOx onto Al2O3 had a significant effect on their reactivity, and the one synthesized hydrothermally at 160 °C was even more active than the Al-Mn complex oxide sorbent reported previously. This work provides a good idea for the design of effective sorbents for NF3 destruction.

- **Keywords:** Destructive sorption of NF3; Al2O3 sorbent; Al2O3 @Mn2O3 sorbent; Reactivity; Utilization

Jian Huang, Jieshi Xiao, Xu Yang. *Distributed SFA-CA monitoring approach for nonstationary plant-wide process and its application on a vinyl acetate monomer process*. Pages 1091-1101.

Driven by the nonstationary and large-scale characteristics in the modern plant-wide processes, this paper proposes a weighting matrix decomposition based distributed slow feature analysis (SFA) task. First, the long-term equilibrium relationships between nonstationary variables are explored by CA to transform the nonstationary variables to be stationary. Based on this, SFA monitoring model is built for whole stationary space to extract the dynamic features. Considering the similar features in the monitoring model, the weighting matrix of SFA is decomposed into subspaces to strengthen the interpretation of local process information. Finally, Bayesian Inference (BI) is used to incorporate the results of each subspace to generate a global monitoring statistic. The effectiveness of the proposed method is tested on the Vinyl Acetate Monomer process.

- **Keywords:** Nonstationary process monitoring; Slow feature analysis; Cointegration analysis; Distributed monitoring; Vinyl acetate monomer process

Hideo Maruyama, Hideshi Seki. *Enhancement of separation rate and recovery efficiency of milk whey proteins by addition of calcium and magnesium ions in batch foam separation*. Pages 1102-1106.

The influence of Ca2+ and Mg2+ to milk whey solution at pH 6 on the enhancement of proteins recovery in batch foam separation was investigated. The pH of whey solution produced in cheese production was about pH 6. The separation rate was evaluated by the separation rate constant, k, by fitting to first-order kinetic equation, and the recovery efficiency was evaluated by the fraction of residual concentration of whey proteins. In the comparison of the case without and with the addition at pH 6, in the case with the addition of Ca2+ and Mg2+ in the range over 0.06 mol/L, the k became 4.4-fold and 2.0-

fold larger, and the recovery efficiency became 5.3-fold and 1.9-fold larger than those in the case without the addition. The overall equilibrium adsorption constant, K, and the overall saturated adsorption density, Xs, were also affected by the addition of Ca2+ and Mg2+. The variation tendency of K and Xs was quite different. As increasing the concentration of both Ca2+ and Mg2+, mostly K decreased, on the other hand, Xs increased. Judging from these results, the formation of aggregates/complexes of whey proteins by the addition of Ca2+ and Mg2+ was suggested. The addition of Ca2+ and Mg2+ could enhance the separation rate and recovery efficiency.

- **Keywords:** Foam separation; Milk whey protein; Calcium; Magnesium; Separation

Meghdad Pirsaheb, Hiwa Hossaini, Anvar Asadi, Zeinab Jafari. *Enhanced degradation of diazinon with a WO3-Fe3O4/g-C3N4-persulfate system under visible light: Pathway, intermediates toxicity and mechanism*. Pages 1107-1123.

In this study, the WO3-Fe3O4/g-C3N4 catalyst was investigated for activating PS in degradation of diazinon under visible light. Characteristics of the synthesized catalyst were analyzed via XRD, BET, TEM, FESEM, EDS, VSM, FTIR and XPS techniques. With the WO3-Fe3O4/g-C3N4-PS system, under optimal conditions (diazinon 5 mg L−1, catalyst dosage 0. 4 g L−1, PS 1 mM, pH 5) a diazinon degradation efficiency of 95% and mineralization of 69% could be achieved after 60 min. The results displayed that the removal of diazinon followed pseudo-first-order (PFO) kinetics, and compared with WO3-Fe3O4/g-C3N4, PS activated with WO3-Fe3O4/g-C3N4 exhibited diazinon removal with higher reaction rate. The quenching experiment confirmed that the main active species were sulfate radicals (SO4·−), hydroxyl radicals (OH•) and singlet oxygen (1O2) and a possible reaction mechanism was suggested. Based on the intermediate products identified by LC-MS/MS, the main reaction pathway was proposed. In addition, the catalyst indicated good reusability after four consecutive experiments. Finally, the by-product toxicity was estimated by the Chlorella vulgaris. This work presented a catalyst with excellent efficiency in the PS activation, implying a new system for degradation of other organic contaminants.

- **Keywords:** Diazinon; Persulfate; Visible-light; WO3-Fe3O4/g-C3N4; Reaction pathway

Di Chen, Chengqing Wu, Jun Li, Kexi Liao. *A numerical study of gas explosion with progressive venting in a utility tunnel*. Pages 1124-1138.

A numerical model of a progressive vented gas explosion is presented. A CFD tool in combination with correlation analysis and an artificial neural network (ANN) were utilized to establish and refine the numerical model. The experimental results of 44 fixed vented gas explosions and one progressive vented gas explosion with moving obstacles were used to validate the numerical accuracy. The results indicated that the method to estimate the activation pressure of the pressure relief panels for a fixed vented gas explosion achieved a lower overpressure prediction compared to that for a progressive vented gas explosion. The progressive venting procedure was modelled by two-layer pressure relief panels with the upper layer having activation pressures with a linear ascent trend. The vents on the tunnel had an insignificant impact on the explosion load after being lifted over the tunnel top, and their falling process was unnecessary to be modelled. A non-negligible impact of the obstacles inside the tunnel on the flow field upon being pushed away from their initial positions was demonstrated. By employing an ANN, the critical parameters in the numerical model were determined, which were used to accurately replicate the experimental results. The findings clarified a revenue for the modeling of a progressive vented gas explosion as well as some shortcomings of the CFD tool.

- **Keywords:** CFD; Gas explosion; Progressive venting; Moving obstacle; Artificial neural network

Balkis Hazmi, Umer Rashid, Sibudjing Kawi, Wan Nur Aini Wan Mokhtar, Thomas Choong Shean Yaw, Bryan R. Moser, Ali Alsalme. *Palm fatty acid distillate esterification using synthesized heterogeneous sulfonated carbon catalyst from plastic waste: Characterization, catalytic efficacy and stability, and fuel properties*. Pages 1139-1151.

The extensive use of plastics in industries and households contributes to the proliferation of plastic waste (PW) in landfills, the oceans, and the environment, which represents a serious threat to numerous fragile ecosystems. Recycling rates for PW are still low, so solutions to the problem of waste accumulation are urgently needed. We report the transformation of waste polyethylene terephthalate food containers into plastic waste char (PWC) via anaerobic pyrolysis and subsequent conversion to an acidic solid catalyst for conversion of palm fatty acid distillate (PFAD) into biodiesel. Such an approach could provide a promising solution to the environmental issue of PW while simultaneously facilitating production of biofuels. In this study, PW was carbonized at 600 °C to yield a carbon precursor that was subsequently treated with sulfuric acid at three sulfonation ratios (1:10, 1:15 and 1:20) to give a series of solid acid sulfonated carbon catalysts, PWC-SO_3H (a), (b) and (c). The synthesized PWC-SO_3H catalysts were thermally stable up to 375 °C. The deposition of sulfonic acid groups onto the catalytic surface was confirmed by infrared spectroscopy. Surface morphology analysis revealed a mesoporous textural structure with random sulfonate group distribution. Changes in crystallinity for PWC and PWC-SO_3H catalysts were determined by x-ray diffraction spectroscopy and supported by Raman analysis. The catalysts were then evaluated for biodiesel production efficacy via esterification of PFAD with methanol. The PWC-SO_3H (b) catalyst (1:15 impregnation ratio) provided the highest yield of PFAD-derived-biodiesel (96.9%) under the optimum reaction conditions of 5 wt% catalyst at 110 °C for 2 h with a methanol to PFAD molar ratio of 18:1. Recyclability studies revealed that the PWC-SO_3H (b) catalyst was reusable for four consecutive reactions while maintaining high catalytic activity. Lastly, the fuel properties of the resulting PFAD biodiesel were within the limits prescribed in ASTM D6751, the American biodiesel standard.

- **Keywords:** Biodiesel; Esterification; Fatty acid methyl esters; Heterogenous catalyst; Palm fatty acid distillate: Plastic waste; Pyrolysis