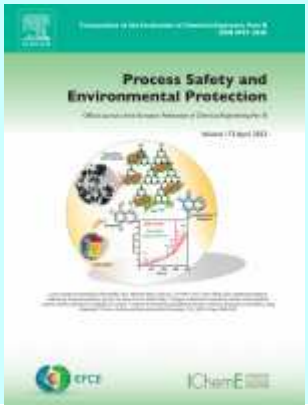
Process Safety and Environmental Protection

Rok 2023, Volume 172

April



Saima Farooq, Rongsheng Cai, James McGettrick, Emmanuel Pean, Matthew Davies, Ahmed S. Al Harrasi, Richard Palmer, Chedly Tizaoui. *Visible-light induced photocatalytic degradation of estrone (E1) with hexagonal copper selenide nanoflakes in water*. Pages 1-15.

Steroid hormones, being potent endocrine-disruptors, are a menace to human health and aquatic life. Herein, visible-light induced photocatalytic degradation of estrone (E1) by hexagonal copper selenide (CuSe) nanoflakes has been reported. CuSe was synthesised by a facile and low-temperature (100 oC) co-precipitation method and was characterised. The nanocrystals were of stoichiometric Cu:Se ratio with Se2- and Cu in the + 1/+ 2 mixed-valence state and exhibited laminar, flake-like morphology with a preferred hexagonal close-packed structure (P63/mmc) having average particle size and thickness of 0.229 ± 0.146 μm and 0.05 ± 0.02 μm, respectively. The adsorption isotherms of E1 were linear and the adsorption process was exothermic. The reactivity of E1 under aqueous suspensions of CuSe exposed to visible light exhibited pseudo-first-order kinetics with a rate constant, k, that varied with initial E1 concentration, light power, catalyst dose, and pH. Particularly, k was almost constant over the range pH5–9 but substantially increased as pH rose to 11, while light power and catalyst dose increased k up to a maximum, and the initial concentration reduced k. Surprisingly, CuSe oxidised E1, even in the absence of light, and leached species that were identified and their time-dependency was determined. We concluded that the disappearance of E1 by CuSe is attributed to synergetic effects of adsorption, oxidation by CuSe, and photocatalytic degradation. Supported by liquid-mass spectrometry analysis and molecular chemistry calculations, we also suggested a possible mechanism for E1 degradation. Thus, hexagonal CuSe nanocrystals can be a promising candidate for the treatment of endocrine-disrupting chemicals (EDC)-contaminated wastewaters.

- **Keywords:** Estrone; Emerging contaminants; Photocatalysis; Adsorption; Copper selenide

J. Treviño-Reséndez, N. Grajales, A. Medel, I. Sirés, Y. Meas. *Generation of hydroxyl radicals in the peroxi-coagulation process with an air-diffusion cathode: Fluorescence analysis and kinetic modeling*. Pages 16-26.

Conventional peroxi-coagulation process is based on the combined occurrence of electrocoagulation and oxidation in a single unit, since H2O2 and Fe2+ are electrogenerated on site from cathodic and anodic reactions, respectively. The present work aims to evaluate the effect of pH and applied current on the generation of hydroxyl radicals (•OH) from Fenton's reaction during peroxi-coagulation treatment. The electrochemical cell consisted of a gas-diffusion cathode with graphite cloth, and an iron plate anode. By using a fluorescence probe (coumarin) and kinetic modeling, it has been possible to estimate the •OH concentration at different current values and to determine the effect of pH on their production. A system with six ordinary differential equations was established and solved to predict the concentrations of the main species of Fenton's reaction. In addition, the interference of possible by-products and side coumarin hydroxylation reactions in the determination of •OH was considered. The simulation results reveal that current increase from 10 to 50 mA positively influences the •OH generation, further decreasing when operating at 70 mA. This is attributed to: (i) the negative effect of an excessive H2O2 generation, and (ii) the increase in pH during the electrolysis. This latter phenomenon is detrimental because of the partial precipitation of Fe2+ catalyst. A sensitivity analysis was performed to determine the most influential kinetic constants of the model on •OH and 7-hydroxycoumarin concentrations. This work demonstrates the importance of considering possible side reactions, which may occur when coumarin is used as a probe compound to quantify the •OH.

- **Keywords:** Fluorescence probe; Hydroxyl radical; Gas-diffusion electrode; Kinetic modeling

Ce Wang, Yuling Lü, Tianxu Ye, Feng Rong, Limin He. *Generation of condensate bubble aphrons (CBA) by partially vaporized condensate to enhance oil removal from produced water*. Pages 27-37.

This paper demonstrates flotation separation for dispersed oil droplets and dissolved organics by preparing condensate bubble aphrons (CBA) by partially vaporizing condensate. The results show that the new CBA consists of a condensate membrane and a gas core, with a three-phase contact angle above 140° from the oil surface due to excellent wettability. At different temperatures and condensate compositions, bubbles are about 25–100 μm in size. The half-life time (140–230 s) of CBA and gas hold-up (10–25%) is much higher than nitrogen bubbles. It shows that the CBA has good stability and dispersibility. The flotation experiment of CBA found that the condensate group distribution ratio was optimally adapted to the temperature, and the optimum oil removal efficiency of up to 87% was obtained when the operating temperature was higher than the bubble point of 25–35 °C. The experimental experiment shown the recommended initial oil concentration (400 mg/L) and the mixing ratio of condensate and water (1.0%). Otherwise, CBA flotation efficiency was 10% higher than dissolved gas flotation. With the addition of flocculant, the CBA flotation efficiency can reach 97% of oil droplets and can achieve 50% removal of Acetic acid (HAc).

- **Keywords:** Bubble properties; Condensate bubble aphrons (CBA); Flotation; Oil-water separation; Partial vaporization

Han Zhang, Jun-Cheng Jiang, Tian-Yi Yan, Lei Ni, Shang-Hao Liu. *Thermal hazard risk and decomposition mechanism identification of 1-Hexyl-2,3-dimethylimidazolium nitrate: Combined thermal analysis experiment and DFT emulation*. Pages 38-47.

Ionic liquids are extensively used in pharmaceutical, chemical and aerospace fields, and sometimes used in high temperature environments. Investigating the pyrolysis hazard characteristics and mechanism of ionic liquids is significant. 1-Hexyl-2,3-dimethylimidazolium nitrate ([Hmmim][NO3]) as a new versatile ionic liquid has been systematically studied in this paper. The pyrolysis characteristics of [Hmmim][NO3] in different conditions are researched by using thermogravimetric analyzer, differential scanning calorimetry and accelerating rate calorimeter technologies. Main thermodynamic parameters, safety parameters, and reaction pattern of [Hmmim][NO3] pyrolysis process are acquired. The severity degree and possibility of [Hmmim][NO3] runaway reaction is evaluated, which may result in serious damage to the plant. The microscopic mechanism of [Hmmim][NO3] pyrolysis has been explored comprehensive utilization thermogravimetry-flourier transform infrared spectroscopy, thermogravimetric-photoionization mass spectrometry and quantum-chemical simulation. The primary noxious gas and reaction steps leading to the thermal hazards of [Hmmim][NO3] are confirmed. This research provides a theoretical basis for improving the intrinsic safety of [Hmmim][NO3] application and formulating corresponding safety preventive measures.

- **Keywords:** Ionic liquids; Pyrolysis hazard characteristics; Microscopic mechanism; Quantum-chemical simulation; Intrinsic safety

Yongnan Zhou, Shiwen Liu, Xiaosai Hu, Yuanyu Ge, Chao Shi, Huanling Wu, Tianchi Zhou, Ziyin Li, Jinli Qiao. *Facilitating the proton conductivity of polyvinyl alcohol based proton exchange membrane by phytic acid encapsulated Zn-azolate MOF*. Pages 48-56.

It is important but still challenging to develop high-performance proton exchange membranes (PEMs) which should meet the following requirements: consecutive proton-conducting channels, efficient proton transfer, and excellent stability. In this study, polyvinyl alcohol (PVA) composite membranes were constructed by loading post synthetically phytic acid (PA) encapsulated Zn-MOF, denoted as PVA@PA@Zn-MOF-X (X = 0, 2, 4, 6. wt%). The novel Zn-MOF with high thermal and pH stability has been synthesized from the zinc salt and dual ligands (H2NDI: 2,7-bis(3,5-dimethyl) dipyrazol-1,4,5,8-naphthalene-tetracarboxydiimide; HBTA: 1 H-benzotriazole) which can be employed to host PA as proton carriers. Composite membranes were evaluated by microstructure, thermal stability, mechanical property, dimensional stability, proton conductivity, and so forth. It is found that the codoping of PA encapsulated Zn-MOF with suitable content is more stability of the composite membranes. Furthermore, PVA@PA@Zn-MOF-4 shows the highest proton conductivity of 1.85 × 10-2 S cm-1 at 80 oC and 90% RH with relatively lower value for ion exchange capacity (0.58 mmol g-1) among the composite membranes. This phenomenon is attributed to the consecutive hydrogen bonding networks which are composed of the carbonyl oxygen sites within Zn-MOF, phosphate groups of PA, and hydroxyl groups of PVA, enhancing the efficiency of proton transport. This is a referable strategy for designing and constructing the high-performance PEMs for fuel cells.

- **Keywords:** Metal organic frameworks; Proton exchange membrane; Phytic acid; Polyvinyl alcohol; Proton transport

Tao Hai, Salar Radman, Azher M. Abed, Ali Shawabkeh, Syed Zaheer Abbas, Ahmed Deifalla, Hadi Ghaebi. *Exergo-economic and exergo-environmental evaluations and multi-objective optimization of a novel multi-generation plant powered by geothermal energy*. Pages 57-68.

An innovative multi-generation energy system is proposed to generate simultaneous power, drinking water, cooling, heating, and H2. The aimed plant comprised of an absorption chiller, a heat pump unit, a reverse osmoses unit, a double flash cycle, and a proton exchange membrane. The devised system is surveyed comprehensively based on the thermodynamic, thermo-economic, and exergoenvironmental indicators for offering an in-depth assessment of the plant. Besides, multi-objective optimization has been employed in the proposed system. The net proportions of output work, unit cost, thermal and exergetic efficiencies, and H2, and purified water production of the system are 99.25 kW, 124 $/GJ, 24.4%, 32.1%, 1.218 kg/h, and 0.9662 kg/s, separately. The outcomes related to thermodynamic and thermo-economic evaluations demonstrate that the greatest amount of total cost rate occurred in the first employed turbine. Owing to the findings of the parametric study, by increasing geothermal temperature, exergoenvironmental parameters are reduced, and with increasing the pressure of FT1, cooling load and energetic efficiency increase while SUCP, net output work, and exergetic efficiency decrease dramatically.

- **Keywords:** Environmental; Geothermal energy; Absorption chiller; Heat pump; Optimization

Matteo Iaiani, Alessandro Tugnoli, Valerio Cozzani. *Identification of cyber-risks for the control and safety instrumented systems: a synergic framework for the process industry*. Pages 69-82.

Malicious interferences to Industrial Automation and Control Systems (IACS) such as the Basic Process Control System (BPCS) and the Safety Instrumented System (SIS) of chemical and process facilities may initiate events with severe consequences such as major accident scenarios (e.g., loss of containment of hazardous substances) and production outages. Existing security vulnerability and risk assessment (SVA/SRA) methodologies, as well as the cybersecurity risk assessment approach proposed by ISA/IEC 62443 series of standards, do not provide any practical method or guideline supporting cyber-risk identification. Moreover, an evident lack of procedures addressing the concrete connection between malicious manipulations of the BPCS and SIS and the impacts on the physical process system that can be initiated, is present in the scientific literature. Given the outlined gap, in the present study, a synergic framework of tools is described and applied to a case study (offshore Oil&Gas platform for gas compression), supporting the systematic identification of the risks that can originate as a result of a malicious interference to the BPCS and SIS. The framework consists of a past incident analysis (PIA) and of two rigorous methodologies, PHAROS, focused on major accident hazards, and POROS, addressing also operability issues. The concept of cyber-attack credibility is here introduced to identify the most credible sets of manipulations based on the score of the plant knowledge level required by the attacker and that of the cyber complexity of the attack pattern, allowing to provide valuable information on how to effectively allocate resources for a more secure network architecture.

- **Keywords:** Cybersecurity; Cyber-risk identification; Chemical and process industry; Major accident hazard; Operability; Systematic methodology

Nonglak Boonrattanakij, Suthinee Puangsuwan, Anabella C. Vilando, Ming-Chun Lu. *Influence of coexisting EDTA, citrate, and chloride ions on the recovery of copper and cobalt from simulated wastewater using fluidized-bed homogeneous granulation process*. Pages 83-96.

Copper and cobalt from industrial operations build up in the environment, posing a substantial health risk. This study examined how ethylenediaminetetraacetic acid (EDTA), citrate, and chloride ions affected the fluidized bed homogeneous granulation process' (FBHGP) ability to recover both individual and combination of copper and cobalt ions from simulated waste streams. A 99% copper removal and 95% granulation efficiency were attained in copper-based solutions. The soluble copper still present in the solution caused a 4% variation in the removal and granulation efficiencies. There were 99% removal and 99% granulation efficiencies in cobalt-based solutions. When EDTA was present in a copper-based solution, 95% removal and 86% granulation were reached, and for cobalt-based solutions, 95% and 91% were the removal and granulation efficiency, respectively. The presence of citrate in the copper-based solution obtained the removal of 83% and granulation efficiency of 54% at 0.1 MR of citrate to copper. No copper phosphate precipitate was formed when the MR was greater than 0.1. There were 96% removal and 92% granulation efficiency when citrate was present in cobalt-based solutions. The presence of chloride ions in copper solution achieved a 99% removal and 91% granulation efficiency, while in cobalt solutions, 99% removal and 98% granulation efficiency were attained. Solutions with combined copper and cobalt with chloride ions achieved 99% removal and 95% granulation efficiency for copper and 99% removal and 95% granulation efficiency for cobalt. The granule sizes decreased as the MR of the complexing agents to metal, and the concentration of chloride ions increased. The peaks on the XRD pattern exactly matched the peaks of cobalt phosphate hydrate ($Co_3(PO_4)_2 \cdot 8 H_2O$). FBHGP has effectively recovered copper and cobalt from the waste streams of simulated metals.

- **Keywords:** Copper phosphate; Cobalt phosphate; Ethylenediaminetetraacetic acid; Citrate; Supersaturation; Chloride ions

Liang Hu, Hailong Yu, Xiaohan Yan, Yunlan Sun, Baozhong Zhu. *Analysis of molten slag from high-temperature plasma treatment of oil-based drill cuttings*. Pages 97-104.

Traditional methods of disposing of oil-based drill cuttings do not provide the much-needed benign treatment. In this study, a skid-mounted thermal plasma processing device was developed with a designed maximum processing capacity of 0.8 kg/min. When the input power of the plasma torch is 10–50 kW, the temperature measured by the thermocouple is 385–1979 °C. After plasma treatment, the morphology of oil-based drill cuttings changes from jelly-like to vitreous state solid structure, and the content of organic matter decreases with the decrease in weight. Mass and volume reductions of 40.98–61.49% and 25.02–68.81%, respectively, were achieved in a treatment period of 0.5–3 min. The total organic compound reduction of 73.08–98.12% was equally achieved in the same treatment period. Due to the special structure of the glassy state residue, the leached concentration of toxic metals is far below the Chinese standard for landfill leachate discharge. This effectively solves the problem of secondary pollution of solid waste. Therefore, thermal plasma technology is an effective alternative method to treat oil-based drill cuttings.

- **Keywords:** Plasma; Oil-based drill cuttings; Molten slag; Toxic metals leaching concentration

Tobias Klöffel, Diana Gordon, Stanislaw Popiel, Jakub Nawala, Bernd Meyer, Pawel Rodziewicz. *Understanding the mechanism of the sulfur mustard hydrolysis reaction on the atomistic level from experiment and first-principles simulations*. Pages 105-112.

After World War II, the Baltic Sea was contaminated by dumping unused sulfur mustard (SM) and other chemical warfare agents (CWAs), which now constitutes a huge environmental hazard. We use both experimental and theoretical methods to understand the reactivity of SM in water, in particular the hydrolysis, which is one of the chemical reactions leading to the neutralization of SM. Real conditions present in the Baltic Sea are represented by performing Car-Parrinello molecular dynamics simulations for sulfur mustard in explicit water solution at finite temperature. We study the relative occurrence and stability of various SM conformers in water and analyze the solute–solvent interactions, with special focus on the formation of intra- and intermolecular hydrogen bonds and their lifetime. A missing piece toward the understanding of the sulfonium cation formation and SM hydrolysis reaction is provided by obtaining the activation energy for SM decomposition in water solution from gas chromatography–mass spectrometry (GC-MS) experiments. The complex mechanism of SM hydrolysis is also studied by umbrella sampling simulations to obtain the free energy barrier for the sulfonium cation formation and to provide an atomistic view of the reaction process.

- **Keywords:** Sulfur mustard; Bis(2-chloroethyl) sulfide; Chemical warfare agents; Car-Parrinello simulations; Gas chromatography

Wen Nie, Yilong Zhang, Lidian Guo, Xu Zhang, Huitian Peng, Dawei Chen. *Research on airborne air curtain dust control technology and air volume optimization*. Pages 113-123.

The mechanization ratio of coal mining faces has reached more than 90%. However, the coal dust pollution in the fully mechanized mining operation is still an urgent problem to be solved, especially in the working area of the shearer driver. Therefore, an airborne air curtain dust control technology is proposed. The air current migration and dust pollution diffusion in a working face under various air volumes were studied using CFD numerical simulation technology. It was found that two high-speed air curtains form at the shearer driver's operating position, while a trapezoidal full-section clean air chamber formed at the sidewalk, which could effectively block the dust engendered by the coal cutting drum. The air curtain with 90 m3/min air volume has the best dust control effect in this area, and the diffusion distance of high concentration dust is reduced by 90 m. After applying this technology in the field, the dust concentration in the shearer driver's working area was reduced to 79.23 mg/m3, and the dust control efficiency was 83%. It is proved that the technology can reduce the dust concentration in the whole tunnel, especially at the shearer driver operating point. This work provides valuable information for dust prevention and control in a working face.

- **Keywords:** Fully mechanized mining face; Airborne air curtain to control dust; Optimal air volume; Numerical simulation

Zhenjun Tian, Qi Jing, Shuo Qiao, Wenhui You. *Encapsulation/capture of S-nZVI particles by PANa-PAM hydrogel limits their leakage and improves Cr(VI) removal*. Pages 124-135.

Sulfide-modified zero-valent iron (S-nZVI) has been shown to be an effective material for removal of various contaminants from wastewater. However, the release of this powder material into the environment brings some hidden troubles to its application. Therefore, poly(sodium acrylate)-poly(acrylamide) (PANa-PAM) hydrogel was used in this study to capture S-nZVI particles within their frameworks, and encapsulate them from being

released into the environment. The structure and composition characterization of the composites (S-nZVI@H) showed that the S-nZVI particles were tightly encapsulated by the cross-linked network frameworks of the PANa-PAM hydrogel. The content of Fe in S-nZVI@H was 123.77 mg/g, and only 6.34% were leached out after being used three times in a row. The maximum removal capacity of Cr(VI) by S-nZVI@H was 9.24 mg/g. Moreover, S-nZVI@H showed excellent reusability and stability. The proposed mechanism of Cr(VI) removal by S-nZVI@H can be described as uptake-reduction-codeposition. The synergistic effect of PANa-PAM hydrogel and S-nZVI particles realized stabilization and solidification of Cr(VI). These results demonstrate that the encapsulation of S-nZVI particles by PANa-PAM hydrogel not only limited their leakage to the environment, but also facilitated the removal of Cr(VI).

- **Keywords:** Sulfide-modified nanoscale zero-valent iron; Poly(sodium acrylate)-poly(acrylamide) hydrogel; Nanoparticles-hydrogel composites; Adsorption

Hongwei Ren, Yize Liu, Ruoyao Zhang, Tengda Zhao, Jing Han, Zhiyang Zheng, Erhong Duan. *Investigation of the CO2 capture behavior in multiple-site natural deep eutectic solvents*. Pages 136-143.

The sustainable development of carbon dioxide (CO2) resource requires the realization of green and efficient capture for the fossil fuel CO2. However, the high operation costs and biological toxicity have hampered the application. Natural deep eutectic solvents (NADESs) are efficient and green CO2 absorbent. In this manuscript, kinds of amino acid-based NADESs were prepared successfully to improve the absorption efficiency of CO2 capture solvent. The chemical structure of NADESs was characterized, and the thermal stability was also measured. The CO2 capture behavior of amino acid-based NADESs was investigated. With multi-reactive sites, unstable stage and more accessibility of alkyl structure on HBA (alkyl amino acids and aromatic amino acids, especial L-Ary), and less electronegativity on HBD (EG), L-Arg/EG NADESs had lower solvation effect (β value, 1.286) and reduced viscosity (48.33 mpa.s at 60 ºC). It behaved better absorption capacity. The optimized conditions by single-factor analysis and Response surface methodology were L-Arg/EG at the mole ratio of 1:5, 30 °C and 200 mL/min, and the absorption could reach 0.81 molCO2/kgNADESs. Additionally, an insight into the reaction mechanism was investigated. It was found that hydrogen-bond structure played an important role in CO2 capture. The broken of H-O···H-N formed by amino acids and ethylene glycol promoted the formation of new bonds of -(O=)C···NHR between L-Arg/EG and CO2, thus achieved higher CO2 capture. The investigated proved that the green solvent amino acid-based NADESs could be efficient absorbents for CO2 capture.

- **Keywords:** Fossil fuel CO2; Capture; Natural deep eutectic solvents; Amino acid

Min Qin, Kexi Liao, Guoxi He, Tengjiao He, Jihui Leng, Shijian Zhang. *Quantitative risk assessment of static equipment in petroleum and natural gas processing station based on corrosion-thinning failure degree*. Pages 144-156.

Quantitative risk assessment method for station static equipment based on the degree of corrosion-thinning failure is proposed. The corrosion rate and failure consequences are divided into 5 severity grades. A corrosion-thinning risk assessment matrix is established. The method is based on the corrosion-thinning intrinsic safety of the petroleum and natural gas process station and avoids the risk evaluation error caused by the mismatch of the failure database. It can analyze the severity of corrosion thinning, which is the improvement of the existing risk assessment method for static equipment. The quantitative risk assessment is applied to DA treatment station in T Oilfield.

Combined with the current status of operation and management of the station, it is determined that the risk level of corrosion and thinning failure is medium.

- **Keywords:** Oil and gas station; Corrosion; Thinning; Risk quantification

Mi Yan, Xiaoqiang Wen, Yansong Sun, Zhihao Zhou, Jiahao Jiang, Ruixiong Hu, Yan Zhang, Dwi Hantoko. *Fly ash treatment by desalination couples with solidification of heavy metals*. Pages 157-164.

Fly ash is the solid by-product of waste incineration. It contains high content of soluble salts and heavy metals, which causes difficulty in treatment. In this study, desalination coupled with heavy metal solidification is investigated for the treatment of fly ash from hazardous waste incineration. The distribution of salt and heavy metal and the leaching toxicity of heavy metal were detected. Sintering not only reduces the bulk density of fly ash but also can reduce heavy metal leaching toxicity. For instance, the soluble heavy metal was reduced by 95.4% after 700 °C sintering. The bulk density of fly ash increases from 0.295 g/cm3 to 1.046 g/cm3 after treatment, which significantly save the space of landfill. Meanwhile, the treated ash can meet the leaching limit of heavy metals for the flexible landfill in China. This research is meaningful for fly ash treatment industry and the sustainable development of waste incineration industry.

- **Keywords:** Fly ash; Sintering; Desalting; Solidification; Heavy metal

Yong Chen, Tianbao Zhang, Feiyu Long, Ruojun Wang. *Methodology for describing the whole process to accident based on entropy increase principle and Darwin's Natural Selection*. Pages 165-183.

The whole process to an accident contains three components including power, origin, and intermediate. Existing accident models always fail to explore the process well. In this paper, a system is considered to be powered by the nature of spontaneous disorder determined by Entropy Increase Principle. The origin is identified as social factors through reviewing the literature regarding hierarchical levels of accident causes. Intermediate is elaborated within the framework of Darwin's Natural Selection. In intermediate, each type of unsafe factors have to struggle with both other unsafe factors and 10 types of safe factors. The unsafe factors which fail to be controlled before an accident occurs must have at least one of variations including latency, mildness, and tendency when they evolve every time. Finally, based on a case study, a comparison is made with Fuzzy Analytic Hierarchy Process. The results from that demonstrates the advantages of the proposed accident model.

- **Keywords:** Entropy Increase Principle; Darwin's natural selection; Accident model; Whole process

Tomaso Vairo, Davide Cademartori, Davide Clematis, Maria Paola Carpanese, Bruno Fabiano. *Solid oxide fuel cells for shipping: A machine learning model for early detection of hazardous system deviations*. Pages 184-194.

With rising concerns about the amount of pollutant emissions generated by shipping and the consequent pressure to curb the environmental impact of shipping activities, fuel cells are expected to take an important role in ship propulsion. In particular, Solid Oxide Fuel Cells (SOFCs) are envisaged to provide high electrical efficiency and offer the opportunity of combining heat and power production. This work deals with the safety issues related to the safety implications of the use of Fuel Cells in maritime applications. A machine-learning model for identifying and intercepting critical events, based on the early detection of the system weak signals, is developed and applied to a Solid Oxide

Fuel Cell (SOFC) system. The model relies on a hybrid approach: a data-driven model based on gradient-boosted decision trees and a computational model of the SOFC system are integrated to enhance the data-driven approach by implementing physics-based knowledge to boost the resulting predictive capabilities. The outlined approach even if it requires further validation at the full scale may be considered a step forward in enabling the prediction of the conditions that may lead to an accident with remarkable accuracy.

- **Keywords:** Early detection; Energy transition; Hydrogen safety; Physics-informed machine learning; Solid Oxide Fuel Cells

Yanfei Xie, Danxia Wang, Sattam Fahad Almojil, Abdulaziz Ibrahim Almohana, Abdulrhman Fahmi Alali, Yihui Zhou, Amir Raise. *CaO-MgFe2O4@K2CO3 as a novel and retrievable nanocatalyst for two-step transesterification of used frying oils to biodiesel*. Pages 195-210.

In this study, biodiesel was generated from used frying oil (UFO) in the presence of CaO-MgFe2O4 @K2CO3 as a novel and effective nanocatalyst. Structural and morphological properties of CaO, CaO-MgFe2O4, and CaO-MgFe2O4 @K2CO3 nanocatalysts were evaluated by EDX/SEM, BET, FTIR, TEM, DLS, VSM, and XRD analyses. Also, life cycle assessment and reaction mechanism were investigated. The utmost biodiesel yield using CaO and CaO-MgFe2O4 @K2CO3 nanocatalysts was acheived 93.55% and 96.53%, respectively, at a alcohol/oil ratio of 15:1 for CaO and 18:1 for CaO-MgFe2O4 @K2CO3, catalyst percentage of 4%, temperature of 70 °C, and reaction time of 5 h, which indicates a significant increase in the biodiesel yield of CaO-MgFe2O4 @K2CO3 compared to CaO. Also, physical features of biodiesel such as density, viscosity, flashpoint, cetane number, pour point and cloudpoint were 882 kg/m3, 4.4 mm2/s, 168 ºC, 58.82, 3 ºC and − 2 ºC, respectively, which are within international standards. Moreover, thermodynamic and kinetic behaviors of transesterification were studied and the results showed that the biodiesel generation process using CaO-MgFe2O4 @K2CO3 is endothermic (ΔH°= 61.9 kJ/mol) and non-spontaneous (ΔG°>0). The activation energy of the transesterification reaction was 64.62 kJ/mol, showing the significant potential of the catalyst in the transesterification reaction. Besides, the reusability of CaO-MgFe2O4 @K2CO3 nanocatalyst showed that it can be used in 4 reuse cycles with high biodiesel yield (>90%). Life cycle assessment showed that CaO-MgFe2O4 @K2CO3 has less negative impacts on the environment than common catalysts such as KOH and NaOH. Also, collecting UFO and using it in biodiesel generation helps to reduce environmental pollution.

- **Keywords:** Biodiesel; CaO-MgFe2O4 @K2CO3; Life cycle assessment; Mechanism; Recyclability; Transesterification

Chao Zhang, Yunhui Zhang, Yangyang Xia, Hongyuan Fang, Peng Zhao, Cuixia Wang, Bin Li, Yanhui Pan, Zhihui Zou, Timon Rabczuk, Xiaoying Zhuang. *Risk assessment and optimization of supporting structure for a new recyclable pipe jacking shaft during excavation proces*. Pages 211-224.

Pipe jacking shaft is an important part of pipe jacking construction, its support structure can support the soil around the pipe jacking shaft to prevent soil destabilization and collapse and ensure construction safety. Most of the existing support structures of pipe jacking shafts are made of cement materials, which have the advantages of high bearing capacity, good integrity and easy access to materials, but also have inherent disadvantages such as high construction cost, long construction period, difficulty in dismantling, and inability to reuse demolition waste, which are not conducive to the sustainable construction. Based on the concept of sustainable construction, this paper proposes a reusable support structure for pipe jacking shafts, which is made of H-shape

steel, steel plate and water stop by welding or bolting assembly, easy to install and disassemble, and can be recycled and reused. In order to verify the bearing performance of the new support structure and evaluate the risk of destabilization during excavation, finite element numerical simulation and full-scale test were carried out, and gives the safety design parameters of new supporting structures by using orthogonal tests. The results show that the finite element numerical simulation results are basically consistent with the full-scale test results, further proving that the numerical simulation results can be used to guide the design and construction feasibility of the support structure during the excavation of the pipe jacking shaft. The construction machinery has a great effect on the safety and stability of the support structure during excavation, and the distance between the construction machinery and the pipe jacking shaft should be reasonably controlled to avoid the risk of structural instability. The results of the sensitivity analysis show that the steel type of the support structure and the spacing of the piles are the two most important factors, which play a key role in the safety and stability of the support structure and should be highly noted in the design and calculation process.

- **Keywords:** Recyclable supporting structure; Finite element simulation; Full-scale test; Risk assessment; Design optimization

Junheng Liu, Xuchao Zhang, Yuan Liu, Ping Sun, Qian Ji, Xidong Wang, Zhipeng Li, Hongjie Ma. *Experimental study on in-cylinder combustion and exhaust emissions characteristics of natural gas/diesel dual-fuel engine with single injection and split injection strategies*. Pages 225-240.

On a non-road, high-pressure common-rail engine, natural gas/diesel dual-fuel (NDDF) combustion mode was performed. The way natural gas energy substitution percentage (ESP) and pilot diesel injection timing affected the combustion process, emission properties and fuel economy regarding NDDF engine with single injection strategy and split injection strategy was experimentally investigated at 25% load of 1800 rpm. Results show that under the two injection strategies, as ESP increased, NDDF combustion altered from single-stage to two-stage slowly, the combustion center (CA50) was delayed, the combustion duration increased, the soot and NO emissions declined, and the brake thermal efficiency (BTE) presented an increase-to-decrease change trend. As the combustion phase of split injection strategy was wholly advanced, the ignition delay period was shortened, the cyclic coefficient of variation (COV) and HC emission declined, and the BTE elevated. Additionally, the advanced injection timing would make NDDF heat release gradually advance, resulting in advanced CA50, extended ignition delay, lengthened combustion duration, lowered unregulated emissions, and increased BTE. The increase in peak heat release rate and BTE of split injection strategy was accompanied by decreased HC and aldehyde emissions. For NDDF engine possessing optimized split injection strategy, the BTE reached 37.79% and the COV reached 1.49% at ESP= 60%.

- **Keywords:** Natural gas; Low carbon combustion; Pollutant control; Split injection strategy; Combustion efficiency; Aldehyde emission

Zhenjie Zhao, Shehong Li, Shilu Wang, Weiqi Lu, Jingan Chen. *Multivariate statistical analysis and risk assessment of dissolved trace metal(loid)s in the cascade-dammed Lancang River*. Pages 241-249.

As a prominent factor impacting water quality, the dissolved trace metal(loid) (DTM) has not been adequately studied in the Lancang River Basin (LRB). Herein, we sampled surface water from 46 sites in the LRB to explore the spatial distribution, primary sources, and associated human health risks of 18 DTMs (As, Ba, Cd, Co, Cr, Cs, Cu, Li, Mo, Ni, Pb, Rb, Sb, Sr, Tl, U, V, and Zn). Affected by geothermal spring input, the concentrations of As, Cs, Li, Mo, Sr, and U were significantly higher in the mainstream

than those in tributaries, with a decreasing trend along the flow direction in the mainstream of the LRB. Tl and Rb are mainly related to naturally derived sources, like soil erosion, Cd, Cr, Cu, Pb, and Zn were mainly attributed to anthropogenic processes, Co and Ni were affected by both natural and anthropogenic processes, while Sb was mainly from the Sb deposit in the basin. As a result of the combined influence of multiple sources of pollution, the spatial distribution of these elements does not seem to be regular. Most of the DTM concentrations in the LRB were within the Chinese and WHO drinking water guideline values, while 43.5% of the samples contained arsenic exceeding the guideline value of 10 μg/L. In general, the water quality of the LRB was good. Health risk assessment indicated that As, Sb, and Tl were the primary drivers of the non-carcinogenic risk. These results give the scientific basis needed for metal(loid) cycling in the aquatic environment and the ecological management of the LRB.

- **Keywords:** Heavy metal; Water quality; Surface water; Health risk; Lancang River

Guanghua Lu, Qi Xue, Xin Ling, Xiqiang Zheng. *Toxic interactions between microplastics and the antifungal agent ketoconazole in sediments on Limnodrilus hoffmeistteri*. Pages 250-261.

Microplastics and personal care products have been identified as two types of emerging contaminants, and their coexistence in sediments may result in interactive effects on benthic organisms. Limnodrilus hoffmeistteri was exposed to polystyrene microplastics (PSMPs) and ketoconazole (KCZ) at different concentrations (0.1–100 μg/g) alone or in combination in sediment-water system for 28 days in this study. Bioaccumulation analysis showed that KCZ in organisms increased with time when exposed to KCZ alone, and the coexistence of MPs significantly increased the accumulation of KCZ in the worms. KCZ and PSMPs alone and in combination decreased the weight of parents and offspring, caused an inflammatory response and induced sediment-avoidance behavior. The activities of antioxidant enzymes in the parents and the activities of detoxifying enzymes in the offspring were activated in response to oxidative stress induced by KCZ and PSMPs. The expressions of endoplasmic reticulum stress related genes (HSP90A, HSP90B, HSP70, HSPA5, PLAA) in the parents and offspring were altered by MPs and KCZ, the offspring showed stronger stress response, and combined exposure seemed to have a synergistic effect on the parents. These findings provide insights regarding the impacts of MPs on the bioavailability of associated pollutants and the interactive toxic effects of these two kinds of pollutants on benthic invertebrates.

- **Keywords:** Microplastics; Ketoconazole; Benthic organism; Bioavailability

Dongyang Qiu, Xianfeng Chen, Lijian Hao, Bo Zhang, Lijuan Liu, Yue Chen, Chuyuan Huang. *Partial suppression of acetaminophen dust explosion by synergistic multiphase inhibitors*. Pages 262-272.

Drug powder explosions pose a potential threat to the process safety of pharmaceutical companies in the processing and storage of products. To explore a reasonable and efficient technology to prevent and mitigate the explosion of combustible drug dust, an experimental system of vertical combustion pipeline equipped with a partial suppression device was built, and the performance of N2 and CO2 loaded with hydrophobic SiO2 encapsulated SiO2 gel (HSESG) respectively to synergistically suppress the explosion of acetaminophen powder was investigated. The results demonstrated that N2/HSESG and CO2/HSESG were effective in reducing the flame average velocity (Vavg), maximum velocity (Vmax), velocity to the top of the pipe (Vtop), and maximum flame temperature (Tmax). N2 loaded with 60 wt% HSESG reduced the Vmax, Vavg, and Vtop of the explosion flame by 68.1%, 66.7%, and 81.3%, respectively, and Tmax by 58.7%. Acetaminophen dust explosion could be completely suppressed by CO2/40 wt% HSESG with 83.7%, 73.0%, and 85.7% decrease in Vmax, Vavg, and Vtop values, respectively,

and 80.7% decline in Tmax. The results of thermal decomposition tests and residues characterization indicated that the partial suppression of N2/HSESG and CO2/HSESG was mainly accomplished through the synergistic interaction among thermodynamic, kinetic, and non-homogeneous chemical effects. Subsequently, the reason for the more pronounced suppression effect under the impact of CO2/HSESG was further explained.

- **Keywords:** Acetaminophen dust explosion; Multiphase composite inhibitor; Partial suppression; Flame suppression; Suppression mechanism

Raquel Greice de Souza Marotta Alfaia, Ronei de Almeida, Kleby Soares do Nascimento, Juacyara Carbonelli Campos. *Landfill leachate pretreatment effects on nanofiltration and reverse osmosis membrane performance.* Pages 273-281.

The present study investigates the effects of landfill leachate pretreatment by coagulation-flocculation (C/F) on the performance of nanofiltration (NF) and reverse osmosis (RO) membranes by comparing permeate flux, fouling resistance, and leachate quality. Pretreated leachates were produced by applying the C/F with ferric chloride (FeCl3) and alum sulfate (Al2(SO4)3), named P1 and P2 leachates. Raw leachate (RL), P1, and P2 samples were treated using five different polymeric membranes termed NP030, NP010, XN45, BW30, and X201. The C/F pretreatment with FeCl3 or Al2(SO4)3 increased XN45's permeate flux by more than 80%. In this case, fouling median resistance values were 2.13e+ 08, 0.96e+ 08, and 1.02e+ 08 m−1 for RL, P1, and P2, respectively. Kruskal-Wallis test showed a significant difference between RL and pretreated leachate groups (p-value < 0.05). No significant difference between P1 and P2 was identified by the Dwass-Steel-Critchlow-Fligner test run for pairwise comparisons. These results indicate that the leachate pretreatment reduced membrane fouling by more than 50%, independently of the coagulant employed. Although higher removals of organic contaminants were, on average, obtained by membrane treatment for RL than for P1 and P2 samples, membranes that operated for RL treatment presented the worst performance in terms of permeate flux and fouling resistance. Therefore, NF and RO processes are not advisable as a single step in a landfill leachate treatment train, and a pretreatment step is recommended. This research makes a major contribution to the field by providing quantitative data for the conceptual premise that leachate pretreatments mitigate membrane fouling. Our findings help elucidate pretreatment effects on membrane performance and determine the preferable leachate treatment layout.

- **Keywords:** Coagulation-flocculation; Fouling; Landfill Leachate; Membrane treatment; Polymeric membranes

Chengtian Cui, Meng Qi, Chi-Min Shu, Yi Liu. *Rigorous dynamic simulation methodology for scenario-based safety analysis of pressure-swing distillation considering independent protections*. Pages 282-304.

Process engineers often assess process safety performance early in the design stage to reduce or eliminate potential hazards cost-effectively. Process simulation tools widely used in design can provide fast and precise hazard evaluation using limited design information. However, there is a knowledge gap on how to build rigorous dynamic process models and how model configurations can affect safety analysis results. This study applied commercial dynamic simulation software, Aspen Dynamics, to address these issues through rigorous dynamic simulations and safety analysis of a two-column pressure-swing distillation with top recycling. The study implements and simulates various layers of protection, including basic process controls, alarms, safety instrumented systems, and pressure relief systems, and evaluates their impact on accident prevention. The hazardous scenarios considered are overpressure and flooding in the distillation columns, and the dynamic responses to a set of deviations such as coolant and steam

utility failures and undesired throughput and composition disturbances are investigated. A scenario-based safety analysis is performed to assess the dynamic safety performance and the effectiveness of protection layers. The results indicate that the presented scenario-based dynamic safety analysis methodology is essential for accurately determining dynamic column behaviors, thereby better assisting in determining process safety time and designing effective safety systems.

- **Keywords:** Process safety performance; Layers of protection analysis; Alarm and safety instrumented system; Scenario-based safety analysis; Process safety time

Ruming Pan, Bachirou Guene Lougou, Yong Shuai, Gérald Debenest. *A multidimensional numeric study on smoldering-driven pyrolysis of waste polypropylene*. Pages 305-316.

The ex-situ smoldering driven pyrolysis reactor can simultaneously remediate the organically contaminated soil/sand and valorize the plastic waste to value-added fuels. This study establishes a multidimensional model to investigate the pyrolysis of polypropylene driven by self-sustained smoldering. The melting and decomposing processes during the pyrolysis of polypropylene have been simulated using the modified apparent heat capacity method and lumped kinetic model. Using a porous structure with high thermal conductivity in the pyrolysis domain proved to be a practical approach to address the non-uniform temperature distribution and low heating rate of plastics during pyrolysis. The research focus of this study is to obtain high-quality plastic pyrolysis liquid (oil, C6–C24) within a reasonable operating time (duration of the plastic pyrolysis process). Also, the operating conditions (Darcy air velocity, initial char concentration, and PP content) determine the yield of pyrolysis products by regulating the temperature and vapor residence time. Therefore, the sensitivity analyses of pyrolysis duration and oil yield to operating conditions have been performed. It is also found that the interface wall (between smoldering and pyrolysis chambers) heat transfer coefficient determines the smoldering chamber's thermal performance. This study provides new insights into the valorization of waste plastics and the remediation of contaminated soil/sand.

- **Keywords:** Self-sustained smoldering; Polypropylene pyrolysis; Multidimensional model; Oil; Value-added fuels

Stewart W. Behie, Hans J. Pasman, Faisal I. Khan, Kathy Shell, Ahmed Alarfaj, Ahmed Hamdy El-Kady, Monica Hernandez. *Leadership 4.0: The changing landscape of industry management in the smart digital era*. Pages 317-328.

This paper strives to identify the significant and unprecedented challenges in loss prevention and process safety facing industry and its senior leaders due to the social / political / economical changes and unrest of the past few years and the threats to world stability. The pandemic with its travel constraints, price hikes, and economic troubles, reinforced by changing energy markets due to the war in Ukraine is threatening global economic stability. This overall situation has introduced a dramatic step change to the conduct of operations for many manufacturers. On top of that comes the threat of climate change and the ongoing energy and digitalization adjustments that industry will have to make to improve socially responsible and to remain competitive in the face of changing expectations. These Industry 4.0 adjustments introduce a great challenge for the management of multinational companies given the greater range of expectations in its operational jurisdictions. Leadership needs to take stock, re-evaluate their business processes and engage resources not tapped in the past to establish a new foundation on which to remain competitive in the future. Within a rather turbulent world, retirement of experienced staff, the multiplicity of several generations working together with their different attitudes and life styles, posed an additional challenge: the need for skilled and

motivated staff to overcome the hurdles. This paper frames these current and future challenges and provides guidance to industry leadership and management to assist in their struggle to meet demands and maintain competitive operations.

- **Keywords:** Corporate leadership; Operating principles; Critical decision-making; Innovation; Learning organization; Dynamic workforce; Skills gap; Education and training; Business continuity; Risk communication; Loss prevention; Business risk; Process safety leadership; Corporate governance; Corporate resilience

Shunling Ruan, Simiao Han, CaiWu Lu, Qinghua Gu. *Proactive control model for safety prediction in tailing dam management: Applying graph depth learning optimization*. Pages 329-340.

Accurate and rapid prediction of monitoring parameters is an important means of proactively preventing safety accidents in tailings dams. Traditional monitoring model uses a single-point time-domain prediction method through feature selection, ignoring the correlation between monitoring point data. Multiple raw monitoring time series were used as direct input to the GCN-AGRU prediction model to estimate response changes in tailings dam operations. Firstly, the spatial location map of sensors in the tailings dam monitoring system was constructed to describe the sensor data in a multi-point arrangement. Then a graph neural network was used to capture the complex spatial dependencies of the sensor location map to obtain the overall safety level of the tailings dam. Secondly, the spatial features extracted from the graph convolutional neural network at different moments were fused with time series and input into a gated recurrent unit (GRU). The purpose was to use the fused features to capture the spatio-temporal correlation between time series of different monitoring locations. Finally, the temporal attention mechanism was combined to predict the dam monitoring data. Based on real data, the algorithm was compared with other algorithms to verify its accuracy and generalizability, which indicates that the model has great significance for improving the risk prevention and control of tailings dams.

- **Keywords:** Graph neural networks; Recurrent neural network; Spatio-temporal data mining; Multi-source data prediction; Tailings dam safety control

Gang Zhou, Jianjun Yao, Qi Wang, Yichun Tian, Jian Sun. *Synthesis and properties of wettability-increasing agent with multi-layer composite network structure for coal seam water injection*. Pages 341-352.

To improve the efficiency of water injection and reduce the amount of dust from the source. In this paper, a wettability-increasing agent with a multilayer composite network structure was prepared. The modified sodium carboxymethyl cellulose (CMC) and linear micelles were rearranged and combined by using the optimal ratio experiment. Through proton nuclear magnetic resonance spectroscopy, Fourier transform infrared spectroscopy, and X-ray diffraction analysis, the functional-group structure and crystallinity of the modified CMC were investigated. The elemental compositions and surfaces of C1 and C2 were examined via energy dispersive spectrometer, optical microscopy, and transmission electron microscopy. A performance test revealed that C2 had excellent temperature shear resistance, and its wettability was good, which was conducive to reduce the spreading of pulverized coal. By observing the coal in dry and wet states, the reason why C2 was suitable for dust reduction was determined. The changes in the functional groups of the soaked coal were analyzed, and the soaking effect of the C2 on the coal was determined. Finally, molecular dynamics simulation was used to verify that C2 played an effective role in promoting moisture wetting of coal.

- **Keywords:** Physicochemical modification; Electrostatic micelle; Coal seam water injection; Infiltration and wettability enhancement; Agglomeration and adsorption

Gholamreza Ahmadi, Ali Jahangiri, Davood Toghraie. *Design of heat recovery steam generator (HRSG) and selection of gas turbine based on energy, exergy, exergoeconomic, and exergo-environmental prospects*. Pages 353-368.

The full repowering of an existing fossil fuel steam power plant is investigated. This study aims to introduce and examine the most important parameters, i.e., the design of the heat recovery steam generator (HRSG) and selection of the gas turbine (GT). The repowered cycle is studied in perspectives of energy, exergy, economic, and environmental views. Considering the pressure levels of the HRSG and the number of HRSGs in the new cycle, six different cases are evaluated. The produced power of the original units is 200 MW. The results of this study show that using two 180 MW GT and two HRSGs results the maximum possible thermal efficiency. By using a high-capacity GT (380 MW), the maximum efficiency will be obtained in case of using one HRSG. Moreover, in all cases, the CO2 production rate is reduced. Introducing new nondimensional parameters named x, y, and α, the balance of the axial force of the steam turbine shaft and the capacity of cooling system are considered. The effect of various parameters on these three parameters are analyzed.

- **Keywords:** Repowering; Thermal power plants; CO2 emissions reduction; Efficiency improvement; Sustainable development; HRSG

Chi-Wen Lin, Yi-Pei Chung, Shu-Hui Liu, Wei Tong Chen, Ting-Jun Zhu. *Optimizing the parameters of microbial fuel cells using response surface methodology to increase Cr(VI) removal efficiency and power production*. Pages 369-378.

Cr(VI) is present naturally as Cr2O72- and its negative charge repels electrons (e-), preventing direct reduction to Cr(III). The Cr(VI) reduction process consumes H+ , suggesting that conventional Cr(VI) reduction techniques a strictly require a low pH, increasing their cost. Therefore, the development of a process that enables Cr(VI) reduction at neutral pH conditions is of interest. In this work, Cu(II) was used as an electron shuttle medium in a microbial fuel cell (MFC). The effects of MFC operating conditions, such as Cu(II)/Cr(VI) ratio, substrate (sodium acetate) concentration and external resistance on the power density (PD) and Cr(VI) removal efficiency were investigated using the response surface methodology (RSM). The maximum Cr(VI) removal efficiency (73%) and power production capacity (30.57 mW/m2) were achieved under pH-neutral conditions with a Cu(II)/Cr(VI) ratio of 1.65, a substrate concentration of 1.36 g/L, and an external resistance of 1360 Ω. The Cr(VI) removal efficiency of the MFC system without added Cu(II) was only 43%, and the power production capacity (15.85 mW/m2) was only half of that under optimal conditions. The removal efficiency of Cu(II) was 100% after seven days. Chromium and copper deposits were observed on the cathode surface, indicating that Cu(II) was deposited on the cathode surface following Cr(VI) removal, eliminating the secondary contamination that is caused by the addition of excess Cu(II). An RSM-optimized MFC system exhibits improved chemical oxygen demand removal, Coulombic efficiency and normalized energy recovery (NER). Its NER is at least 1.5 times higher than that of an unoptimized MFC system, indicating that the MFC most efficiently converts substrates into electrons when the operating conditions are optimized. This work demonstrates that Cu(II) plays a critical role as an electron-shuttle mediator in the removal of Cr(VI). The electron transfer function of Cu(II) increases the efficiency of the reduction that involves Cr(VI), electrons and H+, and eliminates the cost of adding acidic agents, as required in the conventional method in wastewater treatment. The obtained Cu(II)/Cr(VI) ratio is used to determine the maximum amount of Cr(VI) that can be removed by a scaled-up MFC system.

- **Keywords:** Bioelectricity; Cr(Ⅵ) removal; Cu(Ⅱ) addition; Microbial fuel cell; Response surface methodology

Meng Qi, Kyojin Jang, Chengtian Cui, Il Moon. *Novel control-aware fault detection approach for non-stationary processes via deep learning-based dynamic surrogate modeling*. Pages 379-394.

The use of surrogate models for forecasting dynamic behaviors of processes is a promising approach for optimizing process operation and control. This study aims to utilize the powerful prediction capabilities of deep learning-based dynamic surrogate models (DSMs) for fault detection in non-stationary processes, taking into account the impact of control actions on faults. A novel control-aware fault detection approach, utilizing data-driven dynamic surrogate modeling of closed-loop controlled processes, is proposed to detect potential faults under various control actions and operating conditions. DSMs for both one-step and multi-step ahead prediction are developed and combined to detect various types of faults, based on predictions and residuals while considering control effects. High-fidelity dynamic simulations are used to build first principles-based closed-loop process models and generate data under various operating conditions to train the DSMs. Deep learning methods such as long short-term memory and gated recurrent units are employed for dynamic surrogate modeling, and their performance is compared to select the optimal method. The proposed approach is demonstrated through two case studies using a continuous stirred tank reactor and a distillation column with an advanced control structure. The results consistently demonstrate that the approach can achieve both accurate fault detection and reliable false alarm avoidance under different dynamic operating conditions and faulty situations with varying severities and fault types.

- **Keywords:** Control-aware; Fault detection; Surrogate modeling; Deep learning; Dynamic process simulation; Control effects

Meshari M. Aljohani, Salhah D. Al-Qahtani, Mubark Alshareef, Mohamed G. El-Desouky, Ashraf A. El-Bindary, Nashwa M. El-Metwaly, Mohamed A. El-Bindary. *Highly efficient adsorption and removal bio-staining dye from industrial wastewater onto mesoporous Ag-MOFs*. Pages 395-407.

Adsorption is an effective and promising approach for removing pollutants from wastewater. Too many hazardous colors were unintentionally released into the water, which had a negative impact on the environment. A popular textile dye is malachite green (MG). Thus, in this work, an environmentally acceptable inorganic-organic Ag metal-organic framework-based technique to remove colors from industrial water was developed (Ag-MOF). The sorbent was analyzed in the first section of the work using SEM, XPS, XRD, FT-IR, pHpzc, and BET, which confirmed that the Ag-MOF had the BET surface area, is 676 m2/g, which is a significant surface area. In a later stage, the sorption properties of the dye were examined along with the effects of pH, sorbent dosage, temperature, and ionic strength; the sorption isotherms and uptake kinetics were examined: As opposed to the kinetic profile, Isotherm profiles are well-fit by the Langmuir equation and can be modeled by the pseudo-second order rate equation. The outcomes further demonstrated that MG was mostly adsorbed onto Ag-MOF adsorbent by electrostatic attraction forces, hydrogen bonding, ion exchange, and pore filling. 2.25 mmol/g was found to be the greatest adsorption effectiveness of MG onto Ag-MOF adsorbent. (i.e. 809.71 mg/g). Adsorbent dosage, solution pH, temperature, and time were the four adsorption process parameters that were tuned using Box-Behnken design (BBD) in response surface methodology (RSM). The (ΔH°), (ΔS°), and (ΔG°) MG dye was endothermically and spontaneously extracted using Ag-MOF as an adsorbent, according to the specifications. Up to five cycles of adsorption-desorption, the synthesised Ag-MOF adsorbent demonstrates exceptional render ability and cyclability. The produced

adsorbent's efficacy for purifying wastewater samples at a laboratory scale was assessed as a proof of concept. Study the mechanism of interaction between the Ag-MOF and MG as it could be take place through π-π interaction, pore filling, H-Bonding or electrostatic interaction. The mesoporous Ag-MOF adsorbent offered a simple and effective way to handle water filtering and industrial wastewater management. According to our research, this work is the first to explain how to remove MG dye from wastewater samples using Ag-MOF adsorbents.

- **Keywords:** Ag-MOF; Batch adsorption; Isotherm; Thermodynamics; Mechanism of interaction; Box-Behnken design

Chang-Fei Yu, Shang-Hao Liu, Liang Yuan, Dan-Dan Wei. *Thermal decomposition kinetics and mechanism investigation of cumene hydroperoxide under inert gas: A novel experimental method*. Pages 408-416.

Organic peroxides, due to temperature manipulation failure and/or manner disturbances, had been probable to lead to the prevalence of runaway phenomena, even fire, and explosion. Cumene hydroperoxide (CHP), is a traditional liquid organic peroxide for industrial purposes and is applied as a free radical initiator for polymerization reactions in the petrochemical industry. Its utilization in the industrial processes had certain potential safety hazards. In this work, linearly ramped thermal decomposition in CHP was performed using differential scanning calorimetry under a nitrogen atmosphere. Kinetic analysis is made using data from the ramped measurements with two integral strategies (Flynn-Wall-Ozawa and Kissinger-Akahira-Sunose). The gaseous products of thermal decomposition in CHP are investigated via thermal gravimetric evaluation coupled with Fourier transform infrared spectroscopy and gas chromatography/mass spectrometry. Combined with the experimental results, the possible decomposition path of CHP is discussed. This makes up the gap of unclear decomposition mechanism of CHP in inert atmosphere, and has important reference significance for its industrial production and application.

- **Keywords:** Cumene hydroperoxide; Thermal decomposition; Kinetic analysis; TGA-FTIR-GC/MS; Possible decomposition path

Shuai Li, Min Dai, Imran Ali, Hengzhi Bian, Changsheng Peng. *Recovery of nickel from actual electroplating wastewater by integrated electrodeposition with adsorption pretreatment technique*. Pages 417-424.

The rapidly growing electroplating industry has led to the discharge of large amounts of wastewater containing heavy metals. Electrodeposition technique can recover metals from wastewater, however, its application involves high energy costs due to the high levels of inorganic and organic impurities, including metal ions, that are usually present in real effluents. Therefore, in the present work, integrated electrodeposition with adsorption pretreatment technique was employed to recover nickel from real electroplating wastewater in a cost-effective manner. The results showed that adsorption pretreatment technique could simplify the nature of the wastewater by removing 85% of TOC from real electroplating wastewater. Further, the pretreated wastewater was used for electrodeposition and the results indicated that the electrodeposition could reduce the ineffective energy consumption by 50% (from 44 kw·h/kg to 35 kw·h/kg) for actual wastewater, compared to the effective energy consumption of 28 kw·h/kg for simulated wastewater which hinted that the pretreatment by adsorption technique had a positive effect on the deposition of nickel. Analysis of the deposits showed that the recovered nickel was mainly in the form of zero-valent nickel or oxides. The zero-valent nickel adhered tightly to the electrode plates, while the oxide form mainly adhered to the

electrode plates or fell off into the electrolyte. Importantly, the findings of EDS and XRD showed that both simulated and actual wastewater yielded high-purity metallic nickel. Overall, this work provided an effective way to promote the application of integrated electrodeposition with adsorption pretreatment technique for the recovery of precious metals from real electroplating wastewater.

- **Keywords:** Electroplating wastewater; Electrodeposition; Adsorption pretreatment; Energy consumption, Nickel recovery

Lihe Zhu, Fang Yang, Xue Lin, Dan Zhang, Xixin Duan, Junyou Shi, Zhong Sun. *Highly efficient catalysts of polyoxometalates supported on biochar for antibiotic wastewater treatment: Performance and mechanism*. Pages 425-436.

Norfloxacin (NOR), sulfamethoxazole (SMX), and tetracycline (TC) are antibiotics with high residuals in water, which lead to serious bacterial resistance and affect not only the ecological environment but also human health. In this study, heterogeneous polyoxometalate (POM) catalysts of CoPMoV/C was synthesized by cobalt salt, H4PMo11VO40 (PMoV), and biochar from corn stover and then used for activating peroxymonosulfate (PMS) to degrade NOR, SMX, and TC. The strong oxidizing property of PMoV greatly improved the degradation of antibiotics. The optimum removal rate of the CoPMoV/C/PMS system was up to 99.6%, 99.0%, and 100% for NOR, SMX, and TC, respectively. The effectiveness of the reaction system is confirmed by assessing the toxicity of degradation products.

- **Keywords:** POMs; Norfloxacin; Degradation; Peroxymonosulfate

Dongmei Jing, Abdulrazak Abdulsalam Mohammed, Ammar Kadi, Samariddin Elmirzaev, Mohsin O. AL-Khafaji, Mohammad Marefati. *Wastewater treatment to improve energy and water nexus with hydrogen fuel production option: Techno-economic and process analysis*. Pages 437-450.

The use of fresh water to produce green hydrogen fuel through the water electrolysis process can exacerbate the challenges of water scarcity. Using non-potable water for this purpose can lead to the design of a process with high security, reliability and sustainability. This paper develops the conceptual design and techno-economic evaluation of an innovative hydrogen energy production process from a solid oxide electrolyzer (SOE) integrated with a water treatment and recovery process. Accordingly, purified wastewater and waste heat of flue gases of the power plants have been utilized as feedstocks for the electrolysis process. Two different scenarios were assumed to supply the required thermal energy of the electrolyzer: the first scenario is the use of a preheater based on fossil energies, while in the latter scenario the required thermal energy is supplied through parabolic trough collectors, PTCs,-based solar farm. The integrating fossil fuels-driven power plants with evolving green technologies can mitigate the greenhouse gas emission crisis in addition to reducing the limitations of fossil energies. The outcomes indicated that the Levelized cost of hydrogen (LCH) for the second scenario increases by almost 38.7% compared to the first scenario. The reason for the high value of LCH for the second scenario is the high capital cost of solar collectors. Furthermore, the overall conversion efficiency for the proposed hydrogen production process was calculated as 53.26%. The introduced system can be competitive and reliable from the point of view of saving water consumption. The net potential energy saving and carbon emissions of the process was also determined.

- **Keywords:** Wastewater treatment; Water electrolysis; Hydrogen fuel; Techno-economic; Energy and water nexus; Carbon emissions saving

Xiaoliang Ding, Yi Li, Jie Chen, Xingyu Huang, Lu Chen, Zhijun Hu. *Sustainable utilization of finished leather wastes: A novel collagen hydrolysate-based gypsum additive with high-retarding performance*. Pages 451-461.

Finished leather waste is a kind of dangerous solid waste generated by tanneries. Therefore, the effective management of finished leather waste would promote the green and long-term development of the leather industry. In this paper, finished leather waste was selected as raw materials to obtain collagen protein hydrolysate (CPH) with high protein content and then the feasibility study of CPH on gypsum retardation was investigated through comparative analysis with commonly used gypsum retarders. CPH exhibited a satisfactory retarding performance comparable to citric acid (CA) and sodium hexametaphosphate (SHMP), and the retarding performance of CPH on gypsum was gradually enhanced with the dosage increased. Strength measurement and SEM observation indicated that CPH decreased the strength loss of gypsum due to the less impact on gypsum crystals compared with CA and SHMP. Like CA and SHMP, CHP not only featured an effective delay effect on the rise in hydration degree but also changed the hydration heat characteristics in gypsum hydration. The characterization of gypsum hydration product by FTIR and XRD suggested that CPH, CA and SHMP markedly delayed the conversion of gypsum hemihydrate to gypsum dihydrate. Ca2+ concentration determination and XPS analysis further demonstrated that the introduction of retarder altered the chemical environment around calcium element in the gypsum system to delay the participation of calcium ions in the hydration reaction, therefore exhibiting retarding performance. This study reveals a practical and sustainable route for the utilization of finished leather waste, but also provides new theoretical guidance for the development of gypsum additives with high-retarding performance.

- **Keywords:** Finished leather waste; Gypsum retarder; Gypsum retardation; Retardation mechanism

Zhi-Qiang Li, Yiguo Xue, Guangkun Li, Daohong Qiu, Lei Xu, Qiushi Liu, Kang Fu. *Probabilistic determination and application of rock thickness resisting water inrush from karst cave*. Pages 462-472.

Water inrush disaster in karst tunnels is still a challenging topic, and the reasonable thickness of water-resistant rock mass is of great significance in its prevention. This paper proposes a method for determining the thickness of the water-resistant rock mass and its corresponding application flow. First, we encapsulated the frequently used model to calculate the thickness, i.e., the strength model, catastrophe model, and shear model, and anatomized the corresponding factors governing the thickness. Subsequently, the discreteness and uncertainty of rock mass were contemplated by introducing the rock mass homogeneity degree (RMHD). A corresponding calculating process for RMHD was proposed to quantify the distribution and the probability of rock mass parameters with the Weibull function. After that, the quantified probability parameters were brought into the three models to get the thickness and its corresponding probability. The accuracy and applicability of the proposed method are verified and discussed by two typical engineering cases. The results show that the calculation result of the strength model is more in line with the actual reserved value. The thickness obtained by considering the probability parameters of rock mass are well consistent with the actual reserved values. Finally, suggestions for practical application are put forward to distinguish water inrush risk levels and effectively guide the construction as part of safety management.

- **Keywords:** Water-resistant rock mass; Karst tunnel; Probabilistic analysis; Rock mass homogeneity degree; Water inrush

Sheng Qi, Wenjian Wang, Sunyuan Shen, Abdullah Albaker, Madani Abdu Alomar, Ali Rizwan, Arivalagan Pugazhendhi. *Geothermal and solar energy utilization for the development of a sustainable power and cooling production*. Pages 473-485.

The growth of power demand and environmental issues of fossil fuels lead to renewable energy utilization. A novel combination of parabolic trough solar collectors with a double-flash geothermal system is proposed to generate power and cooling simultaneously. Two parabolic trough solar collectors are employed; the first one directly supplies the solar heat during the day and the second one stores the solar heat for the night operating time. Zeotropic mixtures in an integrated ejector refrigeration-organic Rankine cycle are employed to improve waste heat recovery and overall performance. Exergy and exergoeconomic assessment criteria are employed to evaluate the performance of the designed plant. The subsystem's working fluid selection was performed by comparison of the performance of six zeotropic mixtures. The parametric investigation reveals that the exergetic efficiency and net power are affected by the inlet pressure of the separators, and direct normal irradiation presents the highest effect on the payback period. Moreover, the system's optimum state is evaluated by a multi-objective optimization scheme.

- **Keywords:** Double-flash geothermal power system; Parabolic through solar collector; Zeotropic mixture; Cogeneration of power and cooling; Net present value

Mait Kriipsalu, Mohit Somani, Kaur Pehme, Ottar Tamm, Jaak Truu, Marika Truu, Kaja Orupold. *Performance of biocover in controlling methane emissions from landfill: A decade of full-scale investigation*. Pages 486-495.

Methane (CH4) emissions generated from waste management facilities represent a serious global warming concern. The objective of this study was to monitor a fully instrumented biocover capable of abating fugitive CH4 emissions from a closed landfill located at Kudjape, Saaremaa Island, Estonia. This investigation documented the alteration in the emission of CH4, carbon dioxide, and temperature fluctuation for a monitoring period of 10 years after the implementation of biocover. The fine fraction reclaimed from landfill mining along with natural mineral soil and sewage sludge compost in a proportion of 3:1:1 was used as a biocover substrate. CH4 emissions were monitored at the surface and from three locations at a regular depth of 25 cm up to 2 m inside the biocover layer. The measurements recorded from three gas monitoring wells present different scenarios of a typical landfill due to the heterogenous nature of waste and non-homogeneous distribution of landfill gas load to the methane-oxidation layer, namely, a) desired situation where a permanent reduction in CH4 concentration took place over time; b) hot-spot with an extremely high concentration of CH4 albeit consistent decrease over the years; c) a location with minimal initial concentration of CH4. Multivariate analysis showed that the CH4 concentration dynamics and parameters reflecting the CH4 oxidation process activity were different in biocover across the landfill. Based on data analysis results, the CH4 oxidation process stabilizes in biocover in 5–6 years after establishing the cover.

- **Keywords:** Biocover; Landfill Fines; Long-term Monitoring; Methane Emissions

Georges Melhem, Enio Kumpinsky, Joshua Tran, Ronald J. Willey. *An analysis of α-epichlorohydrin-water runaways*. Pages 496-500.

A curiosity began after plotting adiabatic reaction calorimeter (ARC) data from a homework problem placed in a textbook entitled Chemical Process Safety by Daniel A.

Crowl and Joseph F. Louvar, 2011. The data were for a 50/50 mixture (by mass) of α – epichlorohydrin and water mixture. Two exotherms appeared. The first exotherm involved hydration and polymerization of α-epichlorohydrin. A second exotherm appears as well related to the decomposition of reactants and products. Modeling exotherm 1 as a direct hydration of α-epichlorohydrin to glycerin and HCl underpredicted the observed exotherm. Thus, what are the mystery reactions involved that released more energy than predicted by simply modeling hydration to glycerin? This paper reports the answers found to this mystery. A combination of 13 intermediate reactions is proposed.

- **Keywords:** Reactivity; Runaway reactions; Exothermic reactions

Yiqi Liu, Pedram Ramin, Xavier Flores-Alsina, Krist V. Gernaey. *Transforming data into actionable knowledge for fault detection, diagnosis and prognosis in urban wastewater systems with AI techniques: A mini-review*. Pages 501-512.

Recent advances in artificial intelligence (AI) and data analytics (DA) could provide opportunities for the fault management and the decision-making of the urban wastewater treatment systems (UWS) operations. The UWS is typically a large system, including Sewer networks (SNs), Wastewater Treatment plants (WWTPs) and also considering the Receiving media (RM). However, applications of AI and DA in the UWS can be challenging due to the complexities and size of systems, the large variation in the level of UWS instrumentation, and the relatively poor data quality. This review goes beyond the state of the art by critically analyzing previous work on AI-based data-driven methodologies to system-wide fault detection, life cycle fault management and transformation of big and small data into analytics, particularly, considering two different points of view: process faults (such as bulking sludge, sewer corrosion & technology specifics) and instrumentation faults (such as sensors and actuators), thereby offering more opportunities to distinguish complex patterns and dynamics. Our analysis reveals the relative strengths and weaknesses of the different approaches to design fault diagnosis tools and to apply these in the UWS. Finally, the opportunities and challenges about the inter-play among UWS, data and AI are discussed.

- **Keywords:** Fault detection; Fault diagnosis; Fault prognosis; Data analytics; Artificial intelligence

Yu Ling, Biqing Li, Hai Liu, Heping Hu, Yixiao Wu, Biaojun Zhang, Tianyu Zhao, Shaobin Huang, Lishan Niu. *Uncommonly efficient degradation performance of photocatalytic ozonation towards tetracycline over synthesizing 3-D g-C3N4 nanosheet based on Si-O-Co Framework*. Pages 513-522.

3D g-C3N4/Co-MCM-48 was successfully prepared by constructing mesoporous Si-O-Co framework as the template for loading g-C3N4 nanosheet. Excellent synergistic effect and stability in photocatalytic ozonation of tetracycline (TET) were observed owe to the ordered and unique catalyst structure. The results indicated that g-C3N4/Co-MCM-48 possessed better catalytic performance for TET degradation and had an apparent advantage compared with bulk g-C3N4. The highly dispersed Co atoms in the framework acted as reaction centers of ozonation and promoted separation of photo-induced carriers, which further improved the synergistic effect and produced abundant reactive oxygen species (ROSs). Meanwhile, the increase of specific surface area provided sufficient active sites for catalysis. The degradation rate of TET by simulated solar light/g-C3N4/Co-MCM-48/O3 was close to 100% within 8 min, and both the kinetic constant and synergy index of TET degradation were 7.8 and 4.9 times as much as that of simulated solar light/g-C3N4/O3. Effects of various initial pH and Co contents on the TET degradation were studied. In addition, g-C3N4/Co-MCM-48 revealed good stability in

photocatalytic ozonation process by cycling for four times, and the pathway of TET degradation was also proposed in this study. It was suggested that g-C3N4/Co-MCM-48 was an excellent catalyst for the practical application of photocatalytic ozonation.

- **Keywords:** G-C3N4/Co-MCM-48; Photocatalytic ozonation; Tetracycline; Synergistic effect; Reactive oxygen species

Ganesh Shanker Bhandari, Nikhil Dhawan. *Gaseous reduction of NMC-type cathode materials using hydrogen for metal recovery*. Pages 523-534.

The ever-growing demand for rechargeable LIBs in portable electronic devices and electric vehicles has resulted in massive spent NMC-type batteries with the strong urge to recycle these batteries. Hydrogen reduction (pure and mixed gas (10 % H2 + 90% Ar)) of retrieved active cathode powder is investigated for the selective recovery of Li with Ni, Co, and Mn values. The research study was complimented with detailed characterization (XRD, SEM-EDS, XPS, and HRTEM) to analyze the processing mechanism. The thermodynamic evaluation followed by reduction experiments shows the NMC structure dissociation to metal/oxides above 400 °C. The magnetic fraction obtained from water-leached reduced mass possessed a saturation magnetization of 43 emu/g at 500 °C, 60 min containing MnO, Ni, Co, and Li2CO3 in the reduced powder (pure hydrogen) with 91 % Li recovery. Complete decomposition of the NMC structure was observed with 10 % hydrogen gas, but lower Li recovery was seen due to the formation of water-insoluble LiF. Lithium powder (Li2CO3 and LiOH mixture) of ~0.19 kg and ~0.62 kg of magnetic powder containing Co (15.2 %), Ni (38.1 %), and Mn (30.1 %) as MnO can be processed and is economical per kg of cathode powder.

- **Keywords:** Cathode active material; Recycling, Hydrogen; Reduction; Lithium carbonate; Cobalt

Yiming Jiang, Xuhai Pan, Tao Zhang, Zhilei Wang, Xilin Wang, Qingyuan Wang, Yunyu Li, Min Hua, Juncheng Jiang. *Shock waves, overpressure, and spontaneous ignition of pressurized hydrogen in T-shaped tubes*. Pages 535-545.

The accidental release of high-pressure hydrogen into a tube can induce self-ignition, and special tube configurations can complicate their characteristics. Hence, this paper studies the shock waves and self-ignition in tubes with T-shaped structure. Results show that the shock wave intensity decreases after passing through the T-shaped region, and its intensity is lower in the branch pipeline. The flow field is extremely complex after shock waves enter the T-shaped region, accompanied by different shockwave structures (e.g. barrel shock and Mach disk), multiple reflections, and shock-shock interaction. In addition, the location of the bifurcation point affects not only the downstream velocity evolution but also the time of upstream pressure to reach the peak pressure. When the bifurcation point is the closest to the rupture disc, spontaneous ignition is least likely to take place. The flame intensity decreases after passing via a T-shaped zone. Besides, if the T-shaped zone is far from rupture disc, even extinguishment can occur.

- **Keywords:** Hydrogen Safety; Leakage; Flow field; T-shaped tubes; Self-ignition

Hadi Taghavifar, Lokukaluge P. Perera. *Data-driven modeling of energy-exergy in marine engines by supervised ANNs based on fuel type and injection angle classification*. Pages 546-561.

The application of artificial neural networks with the involvement of a modified homogeneity factor to predict exergetic terms from combustive and/or mixing dynamics

in a marine engine is considered in this study. This is a significant step since the mathematical formulation of exergy in combustion is complicated and even unconvincing due to the turbulent and highly nonlinear nature of the combustion process. The computational simulations are carried out on a marine CI (compression ignition) engine and the respective data per different fuel types that are used for thermodynamic exergetic computations as well as energetic simulations. A new parameter namely the modified homogeneity factor derived by an artificial neural network (ANN) is considered for the mixing dynamics, i.e. as an input parameter for the availability and irreversibility predictions. This parameter is based on the standard deviation from an ideal air-fuel mixture formed within the combustion chamber of the marine engine. Furthermore, spray and injection quantities along with the combustion process and its heat transfer parameters are served to predict the exergetic terms for two study cases: (a) fuel type and (b) injection orientation. It is shown that using data analytics that consists of neural networks can provide an adequate approach in diesel engines for improving energy efficiency and reducing emissions.

- **Keywords:** ANN; Engine modification; Exergy; Homogeneity factor; Hydrogen; Marine diesel engine

Weiping Huang, Mohammad Marefati. *Development, exergoeconomic assessment and optimization of a novel municipal solid waste-incineration and solar thermal energy based integrated power plant: An effort to improve the performance of the power plant*. Pages 562-578.

Due to the growing population rate and increasing social activities, the content of municipal solid waste (MSW) production is increasing. Energy production from MSW is one of the promising ways to dispose of waste and reduce the limitations of fossil energies. However, this technology has a relatively low efficiency due to the high volume of moisture and inert materials in MSW and the lower heating value of waste. The integration of solar thermal collectors is one of the suggested solutions to increase the temperature of inlet steam to the power generation cycle in order to improve the power plant performance. In this regards, the present study develops a comprehensive thermodynamic-conceptual and exergoeconomic investigation of the performance of a MSW-incineration (MSWI) plant integrated with a parabolic trough collector (PTC)-based solar field. Accordingly, the temperature of the steam elevates by the solar field before entering the electric power generation cycle. Additionally, the solar unit is integrated with a phase change material (PCM)-based storage system. The use of storage tank at the delivery line of PTC can improve the power plant's reliability. A comprehensive comparison of the developed power plant with the conventional MSWI power plant is presented. In addition, the technical and economic behaviors of the considered power plant have been optimized under two different single and multi-objective optimization scenarios. The outcomes indicated that the developed power plant can provide 15.75% and 15.68% higher energetic and exergetic efficiencies compared to MSWI power plant. In addition, the rate of electric power obtained from S-MSWI power plant is almost 16.1% more compared to MSWI power plant. However, the total cost rate of MSWI plant is almost 24.13% lower compared to the developed power plant. But, the value of LCOE in the developed power plant is approximately 8.93% lower than MSWI power plant. It was also found that, the multi-objective optimization can provide better and optimal results to energy engineers and decision makers compared the single-optimization. The conceptual design of the implementation of the solar field is also developed in a specific geographical condition. Additionally, this research comes from the key technology of the National Key Laboratory of Environmental Protection.

- **Keywords:** Integrated power plant; MSW-incineration; Parabolic trough solar collector; Phase change material; Exergoeconomic; Optimization

Po-Hsuan Yen, Justus Kavita Mutuku, Chung-Shin Yuan, Wei-Hsiang Chen, Chih-Cheng Wu, Chien-Sen Li. *Evaluation of wetting measures and capture efficiencies of fugitive dust emitted from a limestone pile: Experiments and artificial neural network*. Pages 579-587.

In windy conditions, dry bulk material storage sites for limestone fugitively emit dust, causing occupational hazards and posing harmful health effects to nearby residents. According to this investigation, the threshold friction velocity for the limestone was 7 m s−1. As wind speed increases from 7 to 10 m s−1, the concentrations of TSP, PM10, and PM2.5 rose by 148%, 121%, and 76%, respectively. Separate tests were conducted to evaluate fog cannons' and heavy-duty sprinklers' ability to capture TSP, PM10, and PM2.5 and prevent re-suspension from the pile's surface. Eight cases of parameter combinations were investigated, where PM2.5 had the lowest dust capture efficiencies in six instances, while TSP had the highest dust capture in all eight cases. Low spray angles and intermittent water flow regimes showed the best dust collection efficiency. For the fog cannon it was 85.3% and for the heavy-duty sprinkler, it was 79.5%, and they occurred at low and high wind velocities, respectively. The wettability of dust particles smaller than 4 μm in diameter was more difficult than that of larger particles, because the size differences between dust particles and wetting agent's droplets reduces the probability of collision. An artificial neural network was applied to predict dust capture efficiencies from model parameters such as wind speed, spray angle, and water supply regimes. The relative errors in the predicted capture efficiencies for TSP, PM10, and PM2.5 capture were 1.86–4.73%, 2.15–4.57%, and 1.99–6.53%, respectively, implying a good learning ability of the neural network. The results of different wind speed predictions were verified by the F test, where the P values for TSP, PM10, and PM2.5 ranged between 0.17–0.44, 0.18–0.45, and 0.16–0.48, respectively. Overall, intermittent waterflows and low wind speeds optimized the spread of the mist released from the fog cannon, while intermittent waterflows and higher wind speeds were necessary for the optimal performance of the heavy-duty sprinkler.

- **Keywords:** Limestone pile; Respirable PM; Wetting measures; Capture efficiency; Re-suspension; Artificial neural network

Jingjing Liu, Ashkan Bahadoran, Nafiseh Emami, Tariq J. Al-Musawi, Farah A. Dawood, Navid Nasajpour-Esfahani, Iman Najafipour, Seyed Erfan Mousavi, Tiba Ghazuan, Milad Mosallanezhad, Davood Toghraie. *Removal of diclofenac sodium and cefixime from wastewater by polymeric PES mixed-matrix-membranes embedded with MIL101-OH/Chitosan*. Pages 588-593.

Regarding the presence of residual active drug compounds in the municipal effluents and the effluents of pharmaceutical factories, the removal of these compounds increases the resistance of microorganisms, and environmental hazards, such as genetic disorders in the aquatic reproduction and possible damage to human health is necessary. In recent years, using the Mixed-Matrix-Membranes (MMMs) for their high removal efficiency was considered. In the present study, polyether sulfone (PES) membranes, and composite membranes with MIL10-OH/Chitosan (CS), were synthesized and characterized. SEM analysis shows that with the addition of MOF modified with CS, the number and size of micropores and porosity increase compared to the PES membrane. By adding 0.05 wt % of MIL101-OH and MIL101-OH/CS to the PES membrane, the pure water flux increased from 5.1 kg/m2 h to 9.2 and 9.9 kg/m2 h. Increased porosity in the membranes led to a decrease in the resistance of flowing water, and ultimately increased the membrane's permeability. Increased membrane hydrophilicity, as well as membrane surface roughness, reduced membrane clogging. By adding MOF with CS to the PES membrane, the flux recovery ratio increased from 45 % to 95 % in terms of the increase of hydrophilic functional groups of membrane. Furthermore, reversible fouling increases and

irreversible fouling in MMMs significantly decreased. Diclofenac sodium (DCF) was separated better than cefixime (CFX). Thus, the removal percentage for DCF was 95 % and for CFX drug is 90 %. By comparing the removal percentage, it can be seen that the performance of MMMs with MIL101-OH/CS was better than MMMs with MIL101-OH, and adding CS to MOF and PES membrane improved membrane performance to remove DCF and CFX.

- **Keywords:** PES mixed-matrix-membranes; MIL101-OH; Chitosan; Diclofenac sodium; Cefixime

Jinrong Ju, Yali Feng, Haoran Li, Chenglong Xu. *Resource utilization of strongly acidic wastewater and red gypsum by a harmless self-treatment process.* Pages 594-603.

The acidic wastewater and red gypsum generated by the titanium dioxide (TiO2) industry pose a great threat to humans and the environment. In order to achieve low-cost and high-benefit resource utilization of acidic wastewater and red gypsum, a harmless process for the self-treatment of acidic wastewater and red gypsum as well as for the recovery of valuable resources such as Ti, Fe, Ca, and S is proposed in this study. Acidic wastewater was innovatively used to purify red gypsum while reducing its acidity. The results showed that Fe, Ti, Al, Mn, and Mg impurities in red gypsum could be leached efficiently by the acidic wastewater, resulting in the calcium sulfate products, which can be used as a substitute for natural gypsums in industrial production. Subsequently, phosphoric acid was directly added to the Ti-rich filtrate and stirred at 85 ℃ for 45 min, so that the titanium was converted into titanium phosphate precipitation, with an optimal titanium recovery ratio of 94.86%. After recovering Ti, the filtrate was used again to purify red gypsum. Finally, the pH of the low acidity solution was treated by oxidation and precipitation, and filtered to obtain the Fe-rich filter residue and ammonium sulfate solution. The Fe-rich filter residue could be used in the metallurgical industry, and the ammonium sulfate solution was evaporated and crystallized to obtain the (NH4)2SO4 product. The harmless self-treatment process not only facilitated the resource utilisation of acidic wastewater and red gypsum, but also solved the pollution problems caused by wastewater and solid waste in the TiO2 industry.

- **Keywords:** Acidic wastewater; Red gypsum; Resource utilization; Titanium phosphate; Harmless self-treatment process

Mohamed G. Gado, Sameh Nada, Hamdy Hassan. *4E assessment of integrated photovoltaic/thermal-based adsorption-electrolyzer for cooling and green hydrogen production*. Pages 604-620.

An energetic, exergetic, economic, and environmental multicriteria evaluation of the feasibility for an integrated system comprised of an adsorption system and proton exchange membrane electrolyzer operating via photovoltaic/thermal collectors is introduced. The present system produces concurrent green hydrogen, cooling, and hot water under the meteorological conditions of Alexandria, Egypt. The generated electricity from photovoltaic/thermal collectors drives the electrolyzer for hydrogen production. The waste heat from photovoltaic/thermal collectors drives the adsorption unit during summer for cooling purposes, while in winter, it is used for domestic hot water supply. The adopted analysis is built in Simulink and consequently justified with existing literature. The transient variation of temperature profiles, cooling capacity, heating power, COP, input and output exergies, energetic and exergetic efficiencies are investigated. Investigating the daily performance of the adsorption cooling system during the summer exhibits an average daily COP of 0.47 and a system cooling capacity of about 7 kW. The results reported that the adopted system annually yields cooling, heating, and hydrogen of 8282 kWh, 1723 kWh, and 626 kg, respectively. Moreover, it is exhibited that the present system could attain annual energetic and exergetic efficiencies

of 12.3% and 10.6%, respectively. The proposed system demonstrated a substantial payback period of 0.8 years and carbon dioxide mitigation of 52.2 tons. Consequently, combining the photovoltaic/thermal collectors with adsorption cooling systems and electrolyzers could be pronouncedly appropriate for multigeneration systems.

- **Keywords:** 4E multicriteria; Multigeneration; Adsorption system; Hydrogen production and Cooling; Photovoltaic-thermal collector

Mahshab Sheraz, Huyen Ngoc Ly, Van Cam Thi Le, Van Quyet Nguyen, Furqanul Hassan Naqvi, Jin Yong Park, Hojae Lee, Seungdo Kim, Woo Ram Lee, Vijayarohini Parasuraman. *Electrospinning synthesis of CuBTC/TiO2/PS composite nanofiber on HEPA filter with self-cleaning property for indoor air purification*. Pages 621-631.

In this study, we have developed a cure for indoor air pollution. Herein, we have fabricated CuBTC metal-organic framework MOF combined with TiO2 nanoparticle hybrid material by solvothermal method and obtained it in powder form. The CuBTC/TiO2 hybrid material absorbed toluene higher than TiO2 and CuBTC. CuBTC/TiO2 powder hinders its practical application, however, for the first time, CuBTC/TiO2/PS-based nanofibers were electrospun on a commercial HEPA filter using the electrospinning process in order to examine their air-filtering capabilities. This air filter exhibited 98.6% adsorption efficiency and 129.45 mg g-1 toluene gas adsorption capacity, although pristine HEPA was incapable of absorbing toluene. After the saturated point, a self-cleaning strategy was employed under UV light for regeneration purposes. In addition, the CuBTC/TiO2/PS nanofiber demonstrated superior PM2.5 removal performance, with a 99.82% filtration rate. Compared to a pure HEPA filter, the CuBTC/TiO2/PS-C nanofiber-based HEPA filter has a very high filtration rate and negligible pressure drop when evaluated at various airflow velocities. This study gives significant insight into the design of a self-cleaning nanofiber air filter to protect public health from indoor air pollution and save lives in the near future.

- **Keywords:** Indoor air pollution control; CuBTC/TiO2/PS nanofiber; Volatile organic compounds adsorption; Self-cleaning property; PM2.5 capture

Tomaso Vairo, Margherita Pettinato, Andrea P. Reverberi, Maria Francesca Milazzo, Bruno Fabiano. *An approach towards the implementation of a reliable resilience model based on machine learning*. Pages 632-641.

Machine Learning tools to enhance systems' resilience received an increased impetus driven by energy transition, climate change and digitalization, but critical challenges on system requirement definition and reliability of learning processes need to be addressed. This study proposes a systematic framework based on system engineering and focused on the reliability of the learning process of the Hidden Markov Model (HMM) coupled with the Baum-Welsh algorithm. The HMM hidden states may represent the precursors of accidental events, being the states between a regular performance and a failure of a sub-system. The Baum-Welch algorithm, estimating the parameters of the HMM, iteratively updates the estimates of the state transition and observation probabilities. The framework was applied to a real case of LNG bunkering, showing that the system can learn from incomplete data, improve the learning quality given a new set of observations, make predictions about the latent states and enhance system resilience. The novelty of this work lies in ensuring the learning process and contributing to the attainment of an explainable, robust, and interpretable data-driven approach.

- **Keywords:** AI explainability; Energy transition; Learning assurance; Hidden Markov Model; LNG fuel; Plant resilience

Zhenhai Hou, Deming Wang, Wei Zhang, Shengyun Luo, Yansen Lu, Siyu Tian, Qiu Zhong, Zuoming Xu. *Study on the influence of ignition position on the explosion characteristics of methane-air premix in a semi-closed pipeline*. Pages 642-651.

Flammable gas explosion frequently occurs in the actual oil and gas pipeline transportation or mining operations. Given this problem, this paper studies the effect of ignition positions on the explosion characteristics of the methane-air mixture using a semi-closed transparent gas explosion pipe. According to the results, regardless of ignition position, the overpressure curve of each measuring point presents a process of rising-falling to negative-rising-stabilizing, and the flame propagation to the open end (left flame) evolves from spherical to finger shape. As the ignition position is farther away from the closed end, the overpressure at the closed end and the average flame speed on the right side of the ignition source climb gradually. In contrast, the average flame speed on the left side declines gradually. Besides, When the ignition position (IP3 and IP4) are near the open end, P1 (Overpressure at the closed end) overpressure curves under both working conditions oscillate obviously before reaching the peak. The flame front undergoes a repeated compression-stretch-recompression, and the extreme point of the oscillation overpressure waveform always corresponds to the extreme point of the flame position. During this period, the amplitude of the P1 curve grows linearly and parabolically with time. According to the research, the overpressure oscillation is triggered by the reverse pressure wave after the left-side flame rushes out of the pipeline under such working conditions. The growing amplitude during the oscillation can be caused by various factors, including the thermoacoustic instability and the interaction between the flame front of the closed end and the unburned gas column. The research results deepen the understanding of the combustion and explosion characteristics of flammable gas, better the explosion safety protection in its storage, transportation, and processing, and provide a theoretical basis for the safety protection of detonation devices.

- **Keywords:** Ignition position; Methane explosion; Overpressure shock; Flame propagation; Safety

Jie Wang, Yujie Li, Qihui Jiang, Shaoping Tong. *Study on why FeOCl has high Fenton activity in wide range of initial pH and its corresponding stability*. Pages 652-658.

FeOCl was successfully synthesized by partial pyrolysis method and used as catalyst in Fenton-like reaction. The catalytic activity and stability of FeOCl at different initial pH were evaluated in degradation of isoniazid (INH). The experimental results showed that the pH of the solution had an important effect on the catalytic activity and stability of FeOCl. The point of zero charge (pHPZC) of FeOCl was measured to be 1.75. Adding FeOCl could change pH (before addition of FeOCl) of the solution from 3.0, 6.0, 9.0–3.0, 3.9 and 4.4, respectively, being conducive to Fenton-like reaction. The removal rates of INH by FeOCl/H2O2 system at initial pH 3.0, 6.0, 9.0 were 94.48%, 92.45%, 42.32%, respectively. However, degradation efficiency was rapidly degenerative at initial pH 3.0 and 9.0 in stability test. By means of X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM), it was found that the rapid inactivation of FeOCl at initial pH 3.0 was caused by crystal structure transformation of FeOCl into FeOOH and the dissolved Fe, but at initial pH 9.0 was owing to the weakened pH regulation ability of the used FeOCl (only from 9.0 to 6.6).

- **Keywords:** Iron oxychloride; Fenton-like; Isoniazid; Stability; pH value

Chuanrui Qin, Mengtao Dang, Yifei Meng, Dongfeng Zhao. *Fusion calorimetric experiments and QSPR modeling to inversely explore the accuracy of thermodynamic methods: A case study of the apparent activation energies of 18 aromatic nitro compounds*. Pages 659-680.

The choice of thermodynamic analysis method will directly affect the accuracy of thermal hazard assessment. In this work, two advanced calorimetric experiments were used to obtain the pyrolysis parameters of 18 aromatic nitro compounds under dynamic and adiabatic conditions, aiming at the inherent thermal risk and explosion characteristics of aromatic nitro compounds in important chemical processes. The multiple linear regression (MLR) and artificial neural network (ANN) models corresponding to six typical thermodynamic analysis methods (FWO, Kissinger, Starink, Friedman, Townsend, and TMRad) were constructed by using the apparent activation energy (Ea) calculated by fitting as the basic sample data and combining with quantitative structure-property relationship (QSPR). Two kinds of parameters in internal and external validation were used as the main indexes to judge the accuracy and reliability of different kinetic analysis methods applied to aromatic nitro compounds. This study is expected to provide theoretical support and technical guidance for the chemical industry in the thermal hazard assessment process of nitro compounds.

- **Keywords:** Thermodynamic analysis; Quantitative structure-property relationship; Aromatic nitro compounds; Apparent activation energy

Keke Zhi, Zhe Li, Bohong Wang, Jiří Jaromír Klemeš, Lianghui Guo. *A review of CO2 utilization and emissions reduction: From the perspective of the chemical engineering*. Pages 681-699.

CO2 utilization can not only control greenhouse gas emissions but also provide renewable clean energy. CO2 utilization technology is an important technology to control carbon emissions. This work provides a review of CO2 utilization and emissions reduction technology which can provide important theory and a key technology for various applications enhancing cleaner production and carbon emissions reduction. This paper reviews the different areas of CO2 utilization and emissions reduction technology to show the developing timeline and trend of some technology, application scenarios, and development status. The review focuses on photocatalytic technology, synthetic liquid fuel technology, synthetic gas fuel technology, and amine synthesis technology for reducing carbon emissions from the perspective of chemical engineering. Some classic diagrams of key technologies are illustrated, and their characteristics are analyzed. The future direction and potential of chemical engineering include the consideration of feasibility and security in the CO2 emission reduction in a longer period and conclusions made. The efficient use of sustainable energy and the assessment of security risks to human beings are also important areas to be tackled.

- **Keywords:** Chemical engineering; CO2 utilization; Photocatalytic technology; Synthetic fuel; Amine synthesis technology

Wensheng Sun, Shigang Yang, Ya Yang, Qin Fang, Jianlu Zhu, Junhao Dai, Haoyang Li. *Investigation on the concentration prediction model and personnel hazard range of LNG leakage from tankers in the tunnel*. Pages 700-715.

Liquid natural gas (LNG) leaks from tanker in the tunnel could result in more severe fire and explosion catastrophes than those that occur in unconfined space. Investigating the gas concentration distribution law and the accompanying personnel hazard range is crucial to provide guidelines for personnel escape and fire rescue in such accidents. In this paper, to provide a rapid technique for concentration estimation, the virtual source

approach and the fluid settlement theory are applied to put forward a new model, which is based on the Gaussian plume model. Three batches of LNG diffusion tests were carried out in a 5 m long wind tunnel with a cross-section of 1 m × 1 m. The comparison results show that the prediction accuracy of the proposed model in the far region of the leakage source is better than that in the near region, with the error within ±16%, which demonstrated an accurate prediction performance of the proposed model. The numerical model of LNG leakage from tanker in the tunnel is established, and the influence of leakage direction, leakage aperture, and tunnel cross-section on concentration distribution law is discussed. The findings indicate that when the leakage direction changes from horizontal to vertical, the gas is more likely to accumulate in the tunnel due to the greater attenuation of the initial momentum of the gas, which causes the combustible range to increase by about 2 times. When the leakage aperture is 50 mm, the mass of combustible gas reaches the maximum value of 320.91 kg in 85.9 s, which indicates that the explosion intensity is not proportional to the leakage aperture. Excessive leakage aperture causes the concentration to surpass the Upper Flammable Limit, and the similar trends occur when the tunnel cross-section reduces. Based on the numerical results, the calculation model of the personnel hazard range suitable for various tunnel cross-sections and leakage apertures is derived by data fitting.

- **Keywords:** Tunnel; LNG tanker; Gaussian plume model; Wind tunnel experiment; FLACS

Masapogu Yellappa, Omprakash Sarkar, Y.V. Rami Reddy, S. Venkata Mohan. *Municipal landfill leachate remediation coupling acidogenesis and bioelectrogenesis for biohydrogen and volatile fatty acids production*. Pages 716-726.

This study aimed at sustainable treatment of municipal landfill leachate (MLL) along with resource recovery by integrating acidogenesis and bioelectrogenesis. Initially, during acidogenic fermentation, more than 60 % of MLL COD was converted to biohydrogen (0.23 L/g CODload) and volatile fatty acids (VFAs; 56.15 g COD/L). Acetic (25.09 g COD/L), propionic (1.27 g COD/L), and butyric acid (29.77 g COD/L) made up the majority of VFAs. To increase MLL's further treatment, the left-over COD in the acidogenic effluent was introduced into bio-electrochemical treatment system. Three differently configured bio-electrochemical treatment systems (BET1, BET2, and BET3) were evaluated varying their anode composition. BET1 was operated with a capacitive designed PANi/CNT composite electrode, while BET2 was operated with PANi-SSM and BET3 with a graphite electrode. The modified composite electrode in BET1 played a significant role in leachate treatment (COD removal, 71.21 %) displaying a power density of 35 mW/m2. Apart from higher removal of ammoniacal nitrogen, sulfates and phosphates, the composite electrodes in the BET1 resulted in improved bioelectrogenic activity and capacity of electrons migration between electrode and biocatalyst. Additionally, the modified anode showed higher redox peak currents, lower charge transfer resistance, and ohmic losses.

- **Keywords:** Fermentation; Electron transfer; Electroactive bacteria; Landfill leachate

Jiancheng Yu, Baozhong Ma, Shuhe Zhao, Zhichao Yao, Chengyan Wang, Baohua Wang, Minglei Gao, Guosheng Feng. *Vanadium extraction from water-cooled vanadium converter slag via salt-free roasting and acid leaching*. Pages 727-737.

Vanadium extraction from water-cooled vanadium converter slag (VCS) is of great importance for improving the production efficiency of the vanadium industry. A clean process for extracting vanadium from water-cooled VCS is proposed. This process

includes sieving, salt-free roasting, and sulfuric acid leaching. First, through sieving at 100 meshes, large particles of metallic iron are removed and vanadium is preliminarily enriched. Then, salt-free roasting at 950 °C for 1 h can destroy the structures of vanadium ferrospinel and fayalite completely. Vanadate (manganese vanadate, magnesium vanadate, and calcium vanadate), Fe2O3, SiO2, and Fe2TiO5 are formed in the roasted product. Mechanistic analysis shows that as the roasting temperature is increased, oxidation starts from the edges of particles. Vanadium is first oxidized into V4+ and gradually oxidized into V5+. Finally, systematic leaching experiments illustrate that under the optimal conditions, the leaching yields of V, Ca, Mn, and Mg are 94.99%, 89.24%, 46.81%, and 33.11%, respectively, whereas those of Fe, Si, and Cr are only 0.77%, 1.51%, and 1.03%, respectively. Furthermore, phase analysis demonstrates that only vanadate is selectively leached into the solution. The leaching residue does not contain alkali metals and can thus be used as raw material for iron production.

- **Keywords:** Vanadium converter slag; Vanadium extraction; Salt-free roasting; Acid leaching; Mechanism analysis

Melvin Victor De Poures, Damodharan Dillikannan, Gopal Kaliyaperumal, Sathish Thanikodi, Ümit Ağbulut, Anh Tuan Hoang, Z. Mahmoud, Saboor Shaik, C Ahamed Saleel, Asif Afzal. *Collective influence and optimization of 1-hexanol, fuel injection timing, and EGR to control toxic emissions from a light-duty agricultural diesel engine fueled with diesel/waste cooking oil methyl ester blends*. Pages 738-752.

This study attempts to utilize a ternary blend comprising diesel, biodiesel, and 1-hexanol in a direct injection (DI) diesel engine. A response surface methodology (RSM) based optimization with the full factorial experimental design was used to optimize the fuel injection timing and exhaust gas recirculation (EGR) with an objective to maximize the performance of the engine with minimum emissions. Three injection timings and three EGR rates were used. Multiple regression models developed using RSM for the responses were found to be statistically significant. Interactive effects between injection timing and EGR on responses for the blends were studied. From a desirability approach, a HX20 blend (diesel 50 v/v% + biodiesel 30 v/v% + 1-hexanol 20 v/v%) injected at lesser fuel injection timing and EGR rate delivered optimum emission and performance characteristics. Confirmatory tests validated the models to be adequate. With reference to diesel, at optimum conditions, there was a significant reduction in nitrogen oxides (NOx) emission with a marginal increase in smoke, hydrocarbon (HC) and carbon monoxide (CO) emissions. Also, it was found that there was minimal loss in brake thermal efficiency (BTE) of the engine. With respect to waste cooking oil methyl ester operation, the blend reduced nitrogen oxides (NOx), smoke, carbon monoxide (CO) and hydrocarbon (HC) emissions significantly with marginal loss in BTE.

- **Keywords:** Biodiesel; Waste to energy; 1-hexanol; Waste cooking oil; Emissions; Diesel engine

Shuang Liang, Xuechuan Wang, Dongyu Hao, Jin Yang, Xugang Dang. *Facile synthesis of a new eco-friendly epoxy-modified oligomeric chitosan-based chrome-free tanning agent towards sustainable processing of functional leather*. Pages 753-763.

To reduce the contamination of Cr6+ and dyes from tannery wastewater, a chromium-free tanning agent with rich terminal epoxy groups (COS-GTE) was synthesized using oligomeric chitosan (COS) and glycerol triglycidyl ether (GTE). The structural characteristics and application performance of prepared COS–GTE were investigated by FTIR NMR, GPC, SEM, adsorption properties of fatliquor and dyes, and other analysis techniques. The application results indicated that the shrinkage temperature of finished

leather tanned with COS–GTE can reach 83.5 °C. Compared with traditional tanning materials (F-90 and TWS), the finished leather had better mechanical properties (tear strength of 47.410 N/mm2) and yellowing resistance. Moreover, the natural skin modified with COS–GTE showed excellent antimicrobial properties against Escherichia coli, Staphylococcus aureus, Aspergillus flavus, and Aspergillus niger. Especially, the finished COS-GTE tanned leather had a high absorption rate of fatliquor (69.27 %) and dyes (X = 93.21 %), which is beneficial for reducing comprehensive wastewater pollution. The research revealed that the COS–GTE not only can be considered a new biomass material to solve the problem of chromium and dye contamination in the leather industry but also endows leathers with a unique antimicrobial function to extend product protection and service time.

- **Keywords:** Chrome-free tanning agent; Oligomeric chitosan; Antibacterial properties

Xiujie Chen, Yiran Zhang, Jiaqi Ji, Dejun Miao. *Ventilation and cooling of coal mining face based on CFD model optimization*. Pages 764-777.

To solve the problem of high temperatures at the coal mining workings site. The CFD model of the coal mining face was optimized by importing user-defined functions (UDF) in ANSYS-Fluent and simulating the gas-liquid two-phase flow. By analyzing different ventilation variables, an air volume of 36.81 m3/s and an air temperature of 298 K were determined as the optimum ventilation parameters. Based on dynamic multi-field coupling analysis, a spray cooling system was proposed. The influence of water temperature, height, different zones, and spray group spacing on the cooling effect is analyzed by numerical simulation. The results show that the best effect is achieved when the water temperature is 286 K and the group spacing is 10 m. At this point, the peak temperature of a single group on the pavement side is 0.5–1 ℃ lower than the conventional temperature. The maximum temperature was 27 ℃, and the minimum temperature was 24.4 ℃. The effect of the system on cooling is even more pronounced during summer ventilation.

- **Keywords:** Thermal environment of coal mining face; Numerical simulation; Ventilation variables; Dynamic multi-field coupling; Spray cooling system

Xin Zhang, Yuting Huang, Mingjun Bao, Yue Gao, Xiaoxue Zhou, Lexin Liu, Ye Hu, Zhiguang Zhang. *A post-synthetic modified NH2-MIL-125 (Ti) catalyst for boosting photochemical Cr (VI) reduction*. Pages 778-786.

MOFs-based composites with visible light response have gradually attracted wide researchers' attention to water environmental remediation. Herein, a series of post-synthesis modified (PSM) NH2-MIL-125 (Ti) (R-BA-MIL-125 (Ti)) with phenyl-Schiff base-phenyl conjugate systems were successfully synthesized by a simple post-synthetic modification method. Under the optimization of catalyst structure designing, the photocatalytic reduction of Cr (VI) follows the order: –OH > -CH3 > -H > -Cl > -NO2-BA-MIL-125 (Ti) > NH2-MIL-125 (Ti). Among them, 4-hydroxybenzaldehyde-modified NH2-MIL-125 (Ti) (OH-BA-MIL-125 (Ti)) exhibited the highest photocatalytic removal efficiency of hexavalent chromium (Cr (VI)) at visible light conditions and the removal rate for Cr (VI) reached 98.3% under 90 min with only 5 mg photocatalyst, which displayed 2.07 times that of NH2-MIL-125 (Ti). The introduction of para-substituted benzaldehydes not only extended the conjugated chain length, but also subtly reduced the band-gap energy (Eg) of NH2-MIL-125 (Ti). Benefitting from broadening the range of photo-response and enhancing the ability of photoelectron generation, it could significantly enhance the ability of NH2-MIL-125 (Ti) to remove Cr (VI). ESR analyses indicate that e- and •O2- are the main active species. In addition, OH-BA-MIL-125 (Ti) exhibited good reusability and stability over 5 cycles. Therefore, this work will provide

new insights into the fabrication of highly active catalysts by PSM for the remediation of chromium-containing wastewater.

- **Keywords:** NH2-MIL-125 (Ti); Post-synthetic modification; Photocatalytic Cr (VI) reduction; Schiff base structure

Saidatul Hasniza Hasnen, Muhammad Shahid, H. Zabiri, Syed Ali Ammar Taqvi. *Semi-supervised adaptive PLS soft-sensor with PCA-based drift correction method for online valuation of NOx emission in industrial water-tube boiler*. Pages 787-801.

The use of soft sensors for the prediction of Nitric Oxides (NOx) emissions to meet quality regulations has become increasingly attractive from the economic point of view. However, implementation of the standard adaptive PLS soft sensors such as the conventional adaptive block-wise recursive PLS (BW-RPLS) and just in time block-wise recursive PLS (JIT-BW-RPLS) to industrial boilers that are not equipped with an in-line hardware analyzer is impractical. This is due to the limited ability of the adaptive soft sensor to recalibrate without feedback from the actual NOx measurement. Hence, in this paper, a PCA-based drift correction method is proposed for an industrial water-tube boiler in which an in-line hardware analyzer is unavailable. The proposed drift correction factor is used to detect when drift happens and subsequently estimate the corrected NOx value to be used in a semi-supervised manner by the conventional BW-RPLS and JIT-BW-RPLS. Both the proposed semi-supervised BW-RPLS and JIT-BW-RPLS with PCA-based drift correction and estimation methods have displayed an additional 10–20% improvement in prediction accuracy relative to the performance of the conventional supervised BW-RPLS method and 50% prediction improvement compared to offline PLS model, during significant drifts in the industrial boiler operation. All the case studies have been performed using actual industrial data of a water-tube boiler.

- **Keywords:** Partial Least Squares; Adaptive soft sensors; Industrial water-tube boiler; NOx emission; Semi-supervised learning

Andong Yu, Juan Zhou, Min Hua, Xuhai Pan, Juncheng Jiang, Sanming Wang. *Predicting thermal runaway in styrene polymerization reactions: Divergence criterion with phase space reconstruction*. Pages 802-814.

The process of styrene polymerization is a typical hazardous chemical process. Due to its high reaction temperature and high product viscosity, it is very prone to thermal runaway accidents. In order to reduce the occurrence of such accidents, this work investigates the thermal hazard of the polymerization process by reaction calorimetry experiments and deduces the thermal runaway criterion for the styrene polymerization reaction by combining the results of gas chromatography experiments. The phase space of the system was reconstructed by the delayed coordinate method to obtain the reconstructed divergence criterion (re-div). The results showed that the exothermic heat and adiabatic temperature rise of the polymerization reaction showed a logarithmic increase with the increase of the initial reaction temperature. Compared with the div calculated by numerical method and analytical method, the analytical method div is more accurate and effective. The analytical divergence criterion (div) curve is strictly decreasing in the post-polymerization case, which indicates that it can be used as an off-line criterion to determine the safety of the reaction process by the initial reaction condition parameters. After the experimental verification, it can be confirmed that the re-div can predict whether the reaction is out of control in advance and accurately.

- **Keywords:** Styrene polymerization; Thermal hazard; Thermal runaway criterion; Phase space reconstruction; Div; Re-div

S. Madhu, G.M. Lionus Leo, P. Prathap, Yuvarajan Devarajan, Ravikumar Jayabal. *Effective utilization of waste pork fat as a potential alternate fuel in CRDI research diesel engine – Waste reduction and consumption technique*. Pages 815-824.

This work utilized the conventional transesterification process to convert waste pork fat into pork fat biodiesel. The produced biodiesel was meant to serve as a diesel fuel substitution for common rail direct injection (CRDI) diesel engines. Butylated Hydroxytoluene (BHT) as an antioxidant doping with waste pork fat biodiesel-diesel blend has not been analyzed in CRDI diesel engines. Therefore, to improve the ignition process and reduce the engine exhaust emissions in a research CRDI diesel engine, the BHT was employed to combine with diesel-biodiesel mixtures in this work. BHT antioxidants are partially mixed (BHT 50, 100, and 150 ppm) to improve the physicochemical qualities of test fuel and enhance the combustion process of diesel-biodiesel blends (B20). The antioxidant purity was analyzed by energy dispersive X-ray analysis (EDX), structures were analyzed by scanning electron microscopy (SEM) and Fourier transform infrared (FTIR) analyzer spectrograph was utilized to study the biodiesel chemical components. After mixing the BHT, the overall phase of the base fuel remained constant. The experiment outcomes revealed that the biodiesel had higher cylinder pressure than the other test fuels, and the BHT100 ppm blend had a higher heat release rate (HRR). B20BHT100 blend shows 3.98% higher brake thermal efficiency (BTE) at full load operation than pure biodiesel but lowered to diesel fuel. Biodiesel (B100) decreases the smoke opacity by 4.5% compared to diesel fuel. BHT has been incorporated into the biodiesel blend to minimize oxides of nitrogen (NOx) emissions at all loads. The B20BHT150 blend decreased NOx emissions by 5.06% more than diesel fuel at maximum load. Compared to pure biodiesel, the B20 blends reduce carbon monoxide (CO) emissions by 7.1% and hydrocarbon emission (HC) by 12.5%. This research found that adding BHT to biodiesel blends lowers NOx emissions with a slight impact on performance.

- **Keywords:** Antioxidant; Pork fat biodiesel; Butylated hydroxytoluene; Combustion; Emissions

Zhenhai Hou, Deming Wang, Yunfei Zhu, Shengyun Luo, Qiu Zhong, Zhenqi Liu, Yansen Lu, Yabo Zhang. *Experimental study on pressure wave-induced explosion of different types of deposited coal dust*. Pages 825-835.

When the gas explosion occurs in a coal mine, the pressure wave will induce coal dust (CD) to participate in the explosion reaction, which will further expand the accident and eventually cause more serious casualties. Based on this hazard, experiments were performed on three representative types of CD with the aid of a self-built experimental pipeline for gas/CD explosion. The explosion characteristics under the condition that pressure waves entrain different CD to participate in the explosion were studied. Furthermore, the influence of volatile content in CD on the compound explosion was analyzed from a microscopic perspective. The following beneficial conclusions were obtained: The overpressure peak value and the flame propagation velocity in the compound explosion are positively correlated with the volatile content in CD. Under those three conditions, the maximum overpressure is obtained at P2 position, and obvious stratification occurs in the process of flame propagation. However, compared with the other two working conditions, the average flame propagation speed of the composite explosion system with anthracite decreased by 51.2% and 52.6%, respectively, and flame surface breaks and becomes discontinuous earlier. After the explosion, the volatile content of three kinds of CD is significantly reduced, and the volatile content of lignite, bituminous coal and anthracite is 75.6%, 75.7% and 44.7% of the industrial analysis value of raw coal, respectively. With reference to the analysis on the microscopic test

results, the amount of volatile gas decomposed from volatiles determines the intensity of the homogeneous reaction in the whole combustion process, while the coke formed after the reaction determines the intensity of the non-homogeneous reaction. Therefore, the volatile content in CD is a key factor affecting CD explosion. The research results provide an important scientific and theoretical basis for the prevention, control and reduction of CD explosion disasters.

- **Keywords:** Gas/coal dust explosion; Volatiles; Flame morphology; Flame propagation velocity; Explosion overpressure

Aref Shokri, Bahram Nasernejad. *Treatment of spent caustic wastewater by electro-Fenton process: Kinetics and cost analysis*. Pages 836-845.

Spent caustic is a highly contaminated wastewater from critical industries with complicated chemistry and different environmental adverse effects. Conventional wastewater remediation approaches are not effective enough for the remediation of spent caustic. Hence in this study, Electro-Fenton (EF) technology as a subsection of Advanced Oxidation Processes (AOPs) was applied for the removal of chemical oxygen demand (COD) in spent caustic effluent. For statistical analysis and experimental design of each factor including H2O2/COD, current density, pH, and treatment time on the COD removal (response), the Box Behnken Design (BBD) was used. The optimal conditions for operating factors were as the following: H2O2/COD = 0.73, pH= 5.46, current density = 18.83 mA/cm2 and treatment time= 69.88 min. In these conditions, the actual and predicted COD removal was 93.0% and, 94.38%, respectively. Finally, it concludes that Electro-Fenton technology was reliable and outstandingly efficient for COD removal in spent caustic wastewater. The kinetic studies confirmed that the removal of COD tracked the first-order kinetic model and the constant reaction rate and half-life of COD removal kinetic were 0.0257 min−1 and 27 min, respectively. The operating costs analysis showed that the Electro-Fenton process had lower operating costs and it can be a good opportunity for the treatment of spent caustic wastewater on an industrial scale. The operational cost for this process was found to be 1.562$ M−3kg−1COD removal.

- **Keywords:** Electro-Fenton; Cost analysis; Box Behnken design; Spent caustic wastewater, Kinetic studies

Junchao Zhao, Yangyang Fu, Song Lu, Guangbin Lu, Feng Xue, Heping Zhang. *An improved method to determine the minimum extinguishing concentrations of ultrafine dry powder agents: Taking NaHCO3 and KHCO3 as examples*. Pages 846-856.

Ultrafine dry powder agents (UDPAs) are the most potential Halon substitutes due to the high extinguishing effectiveness and excellent environmental friendliness. Nevertheless, the method for obtaining minimum extinguishing concentration (MEC) is flawed and inaccurate. An improved method is proposed by developing the special laser measurement system without powder contamination, the concentration calibration test bench and the cup burner with uniform aerosol generating. The results show that the optimum calibration position is 0.35–0.65 m from the inlet in the y-axis coordinate. More accurate mathematical relationships between the transmittance of the laser measurement system and the NaHCO3 and KHCO3 powders are established, with the errors less than 12%. Upon reaching MECs in the modified cup burner, the flames pulsate, then fade and eventually die. Based on the phenomenon of the sudden change in the transmittance of the laser measurement system at the moment of flame extinguishment, i.e. the "step shape" curve, a more accurate critical criterion point for the MEC is proposed. The measured MECs for methane flames by NaHCO3 (32.2 g/m3) are approximately 4 times that of KHCO3 (8.2 g/m3), consistent with previous studies. The obtained MECs of NaHCO3 and KHCO3 for kerosene flame are verified by 1 m3 total

flooding fire extinguishing experiments. The improved method may guide the design of industry fire protection systems based on UDPAs to achieve process safety.

- **Keywords:** Minimum extinguishing concentration; Ultrafine dry powder agents; Cup burner; Laser transmittance; Calibration

Yue Gao, Yuting Huang, Mingjun Bao, Xin Zhang, Xiaoxue Zhou, Lexin Liu, Zhiguang Zhang, Libin Zeng, Jun Ke. *Ti-doped Zr-UiO-66-NH2 boosting charge transfer for enhancing the synergistic removal of Cr (VI) and TC-HCl in wastewater*. Pages 857-868.

The pollution of hexavalent chromium (Cr (VI)) and tetracycline hydrochloride (TC-HCl) in water environment is considered to be an urgent environmental problem. However, designing and preparing photocatalysts that can effectively remove these contaminants remains a challenge. Bimetallic metal organic framework (MOFs) Ti-doped Zr-UiO-66-NH2 (UiO = University of Olso) Tiα-Zr1-α-UiO-66-NH2 were prepared for the simultaneous removal of Cr (VI) and TC-HCl. The experimental results of photocatalytic performance show that the Cr (VI) removal rate by Ti0.4-Zr0.6-UiO-66-NH2 in single and mixed systems reach 80.9% and 99.8%, which are 1.1 and 1.4 times higher than Zr-UiO-66-NH2, respectively. The BET results confirm that the specific surface area is effectively increased due to Ti doping, which further exposes more reaction active sites. Simultaneously, the MMCT process from Zr to Ti promotes the transfer of photogenerated carriers and suppresses their recombination. The DFT calculation results demonstrate that TiαZr1-α cluster significantly enhances the generation of optical electronics and promoted its transfer. The bimetallic MOF photocatalysts provide a new way for efficient photocatalytic collaborative removal of Cr (VI) and TC-HCl pollutants from wastewater.

- **Keywords:** Bimetallic MOFs; Photocatalytic; Pollutant removal; Metal-to-metal charge transfer; Synergistic effect

Mourad Chebila. *Many-objective robust decision making for efficient designs of safety instrumented systems*. Pages 869-881.

A robust decision making framework is proposed to support the appropriate design and use of safety instrumented systems. This framework incorporates many-objective optimization, uncertainty analysis, robustness assessment, scenario discovery and sensitivity analysis to enhance the decision maker’s confidence in selecting a suitable policy and assessing its ability to perform as required under a wide range of plausible states of the word with a clear definition of any existing limitations and vulnerabilities. For this, the probabilistic behavior of safety instrumented systems is taken into account with detailed presentations and discussions of the needed resources and impacts of employing this kind of safety measures. This included capital cost, recurring cost and many aspects of the associated side effects, which covered loss of production, environmental impacts, and ability to intensify existing risks or even trigger new accident scenarios. A detailed application is provided to illustrate the specificity and the outcomes of each involved step.

- **Keywords:** Industrial safety; Safety systems; Many-objective optimization; Uncertainty analysis, robustness assessment; Scenario discovery

Liuyan Zhou, Yuqing Xie, Xiaowu Wang, Pengbing Li, Yuyue Liu, Zhifang Wang, Jinping Dai, Huitao Zhang, Xinping Yang. *Influence of different microbial inoculants on nitrogen retention and diazotroph community succession during cotton straw composting*. Pages 882-893.

Inoculation with microorganisms is an effective method for promoting compost maturity and quality. This study investigated the effects of different microbial inoculants on compost maturity, nitrogen retention, and the diazotroph community during cotton straw composting. Results revealed that inoculation improved organic matter degradation and compost maturity, increasing the total nitrogen masses by 6.6–33.0% and the total nitrogen by 84.6–112.1%. Particularly, the microbial inoculants containing Anoxybacillus rupiensis, Paenibacillus illinoisensis, and Bacillus velezensis (1:1:1, T1 treatment) exhibited the highest total nitrogen masses and total nitrogen content. Furthermore, inoculation enhanced nitrogenase activity and nifH abundance, and markedly influenced the succession of the diazotroph community, increasing their sensitivity to environmental variables during composting. Furthermore, the total nitrogen, C/N ratios, and moisture content significantly affected the diazotroph community. Results from a network analysis indicated that inoculation affected the co-occurrence patterns among the diazotroph species and increased complexity between diazotrophs. In conclusion, this study provided three promising microbial inoculants for high-quality compost production and a reference for promoting nitrogen retention in cotton straw composting.

- **Keywords:** Composting; Nitrogen retention; Diazotroph community; nifH gene; Network analysis

Jinxi Dong, Zhaosheng Yu, Xikui Zhang, Jiajun Luo, Qihong Zou, Chao Feng, Xiaoqian Ma. *Data-driven predictive prognostic model for power batteries based on machine learning*. Pages 894-907.

Under the pressure of energy and environmental protection, new energy vehicles have become the future direction of automotive development. However, the safety performance of the power battery has always been the most critical indicator in the new energy vehicle industry. The battery will be aged in the continuous charging and discharging cycle, and the aging will cause safety hazards when it reaches a limit. A model that can predict the battery life can be obtained using Machine Learning. To obtain models that can predict power battery life relatively accurately, this paper revolves around the chaos sparrow search optimization algorithm, Random Forest, XGBoost, LightGBM, CatBoost, and NN, the importance assessment of the features, the hyperparameter search process, and the comparison of the differences and performance between the different algorithms are discussed. CatBoost has the highest prediction accuracy, with the amount of predicted data with a relative error of less than 10% being 88.44%. (a total of 10,275 data in the test set). And finally comes up with a general approach to predicting power battery life using Machine Learning.

- **Keywords:** Power battery; Life prediction; CatBoost; Random forest; Machine learning

Jinkun Men, Guohua Chen, Genserik Reniers, Xiaohui Rao, Tao Zeng. *A hybrid deep belief network-based label distribution learning system for seismic damage estimation of liquid storage tanks*. Pages 908-922.

Liquid storage tanks play a vital role in the modern chemical process industry (CPI). The strong ground motion caused by large-scale earthquakes may easily impose severe structural damage on liquid storage tanks, leading to a series of catastrophic cascaded events. The seismic damage estimation of liquid storage tanks is a challenging problem, as the fluid-structure interaction exhibits extremely complicated and non-stationary

response behavior. This study develops a novel data-driven methodology to estimate the seismic damage state probability distribution of liquid storage tanks in the contexts of label ambiguity and data imbalance. With the support of the advanced deep learning framework, synthetic oversampling methods, and label enhancement techniques, a hybrid deep belief network-based label distribution learning system (HDBN-LDLS) is proposed for probability distribution learning. The proposed HDBN-LDLS is evaluated on the widely used ALA database. Simulation results indicate that HDBN-LDLS can achieve a balanced estimation for all damage states while maintaining sufficient robustness to cope with label ambiguity. The reliability of the obtained data-driven model is validated by a damaged tank in the 2006 Silakhor earthquake. For practical applications, a more natural way to estimate a seismic damaged tank is to assign a membership degree to each possible damage state. The proposed methodology can quickly obtain the seismic damage state probability curves of a specific liquid storage tank, which can be used to support quantitative risk assessment and seismic design.

- **Keywords:** Seismic damage estimation; Label ambiguity; Damage data imbalance; Liquid storage tanks; Label distribution learning

Lucie Bartoňová, Helena Raclavská, Jan Najser. *Vanadium – Valuable and toxic element in coal combustion ash: An overview*. Pages 923-940.

The paper evaluates all important aspects related to V present in coal and its behaviour during coal combustion with particular attention paid to its potential extraction from ash and slag wastes. Due to great environmental benefits of co-combustion of coal and wastes, these alternative fuels and corresponding ash and slag counterparts were also taken into evaluation. Specifically, the paper summarizes V levels in world coals, in other related materials (alternative fuels, additives etc.) and in ash and slag residues including V speciation and discussion of its valence states. Theoretically predicted (equilibrium-based) calculations and species are compared with experimental results; due to a significant effect on mitigating CO2 emissions, attention is paid also to oxy-fuel combustion conditions. With the aim to extract V out of the ash and slag residues, physical, chemical, and biotechnological separation methods are discussed in detail along with dominant affecting factors. The paper includes also concluding remarks and highlights the most promising trends and limitations thereby providing suggestions for future research.

- **Keywords:** Vanadium; Coal combustion; Ash; Physical separation; Leaching; Wastes

Alaa Mohamed, Samy Yousef, Andrius Tonkonogovas, Arūnas Stankevičius, Arūnas Baltušnikas. *Fabrication of high-strength graphene oxide/carbon fiber nanocomposite membranes for hydrogen separation applications*. Pages 941-949.

Graphene oxide (GO) is a promising nanosheet for developing next-generation thin-membrane technology to enhance gas permeability and selectivity performance based on the interlayer spacing principle. This study aimed to strengthen GO membranes for enhancing gas permeability and selectivity using non-woven carbon fiber (CF) fabric. The GO/CF membranes were synthesized with 1 wt% of GO and different CF orientations in the matrices with various GO layer thicknesses (200–800 μm). The resulting membranes were characterized for their surface and cross-sectional morphology, pore sizes, mechanical, chemical, and thermal analysis. The SEM results showed successful deposition of GO flakes onto the CF surface with high cohesion with the fibers, accompanied by some deviations in the GO edges, allowing gases to pass through the membranes. In addition, thinner membranes had higher Young's modulus (56 MPa) and surface roughness in the ranges of 84–184 nm. While the gas permeability measurements revealed that the thinner membranes (200 μm) had higher gas

permeability in the range 7809214 Barrer (CO2) and 23154004 Barrer (H2) with an increase of 68–92% compared to the thicker membranes (600 and 800 μm). Moreover, thinner membranes showed higher selectivities about 5.2 (H2/CO2), 4.3 (H2/N2) and 3.6 (H2/CH4). Overall, these results indicate that GO/CF membranes are a promising solution for hydrogen separation due to their high strength and ease of fabrication.

- **Keywords:** Graphene oxide; Non-woven carbon fiber; Gas separation; Hydrogen separation

Juan Jesús De la Torre-Bayo, Montserrat Zamorano, Juan C. Torres-Rojo, Miguel L. Rodríguez, Jaime Martín-Pascual. *Analyzing the production, quality, and potential uses of solid recovered fuel from screening waste of municipal wastewater treatment plants*. Pages 950-970.

Over time, wastewater management evolves into a circular model, producing energy and moving towards zero waste. The usual screening waste treatment is the elimination, with no energy recovery processes. As an alternative, the production of solid recovered fuel (SRF) from screening has been studied, both non-densified and densified, in pellet form. The densification was developed, taking as variables the input moisture and size of the die, obtaining 20 different samples. The optimum pelletizing conditions are an input moisture content of 10% and dies with a compression ratio of 6/20, 6/24 and 8/32. SRF properties have been evaluated based on a quality proposal presented in this paper, which has been developed given the lack of uniformity in the existing SRF standards. The SRF produced complies with fuel quality requirements, such as lower calorific value, with values between 13.37 and 25.65 MJ/kg; Cl and Hg content, with maximums of 0.066% and $1.0 \times 10{-}5$ mg/MJ, respectively; and ash content, between 7.22% and 9.85%. Energy from waste plants could be the destination for all the SRF produced. Its use in cement plants and gasification processes, more restrictive than the previous one, would require manufacturing processes with adequate moisture levels and die size.

- **Keywords:** Wastewater screenings; Solid recovered fuel; Waste to energy; Circular economy; Pellet; Densification

Yuanyuan Xu, Genserik Reniers, Ming Yang, Shuaiqi Yuan, Chao Chen. *Uncertainties and their treatment in the quantitative risk assessment of domino effects: Classification and review*. Pages 971-985.

Domino accidents are typical low-frequency and high-consequence events in chemical process industries. Applying quantitative risk assessment (QRA) in domino accident assessment is challenging due to the uncertainties in the escalation process. Meanwhile, the outcomes of QRA are subject to a certain degree of unreliability due to the inappropriate representation of uncertainty. This paper reviews the literature in the field of QRA of domino accidents that may happen in the chemical process industries. Firstly, the sources of uncertainty in risk assessment of domino effects are identified and categorized based on a fundamental structure of uncertainty and a QRA framework. Furthermore, the current methodologies and approaches applied for handling various uncertainties (input uncertainty, model parameter uncertainty, and model structure uncertainty) in the QRA related to domino effects are reviewed. Based on the literature review results, current challenges with respect to uncertainty handling in QRA of domino accidents are discussed, and recommendations for future research are given before the conclusions are presented. This study helps researchers to get insights into the interface between uncertainty fundamentals and the QRA framework and the current status of uncertainty handling in the QRA of domino effects. Furthermore, this study promotes the development of new approaches for handling uncertainty in domino accident analysis.

- **Keywords:** Domino effects; Uncertainty fundamentals; Quantitative risk assessment; Chemical process industry; Uncertainty handling

Ramadhass Keerthika Devi, Muthusankar Ganesan, Tse-Wei Chen, Shen-Ming Chen, Muthumariappan Akilarasan, Syang-Peng Rwei, Jaysan Yu, Kuan-Yu Lin, Anlin Shaju. *Oxygen-terminated vanadium carbide with graphitic carbon nitride nanosheets modified electrode: A robust electrochemical platform for the sensitive detection of antibiotic drug clioquinol*. Pages 986-997.

Engineering the electrocatalyst's nanostructure is key-factor in constructing a high-performance electrochemical sensor. The MXene vanadium carbide (V8C7Tx; VC) nanosheets encapsulating graphitic carbon nanosheets nanocomposite (VC/g-CN NSs NC) as an effective electrocatalyst for detecting clioquinol (CQL) is reported here. The interconnected VC and g-CN nanosheets form a very effective conductive network. The high concentration of O-terminated functional groups in the oxidized VC and the abundant surface area of g-CN contribute to the enhanced electrocatalytic effectiveness of the nanocomposite. The synergistic interaction between the VC NSs and g-CN NSs creates a nanocomposite ideal for CQL detection because it offers many active sites with a fast electron transfer rate. A lower oxidation potential and higher peak current responsiveness distinguish the proposed drug sensor from previously described CQL sensors. Under optimal conditions, the constructed sensors showed strong analytical performance, as shown by a low detection limit of 2.2 nM, high sensitivity of 15.6 μA μM−1 cm−2, a broad linear range of 0.3–220 μM, and significant recovery outcomes in the analysis of real samples. Thus, the VC/g-CN NSs NC material has promise for use in high-performance electrochemical applications.

- **Keywords:** MXene; Vanadium carbide; Graphitic carbon nitride; Clioquinol; Electrochemical sensor

Ke Guo, Zhengyang Li, Yuequn Cao, Yuling Yang. *How efficient is the environmental pollution control in China?* Pages 998-1009.

Currently, China is at a critical stage of economic transformation and pollution control. The environmental pollution control efficiency (PCE) deserves more in-depth study. This paper adopts a three-stage global data envelopment analysis (DEA) model and a global Malmquist index model to measure the PCE and the sources of its changes in China from 1991 to 2019. Study shows that: (1) the overall level of PCE has remained low over the past 29 years, and it has a slowly fluctuating upward trend, with an average annual growth rate of only 0.92 %; (2) the lower pure technical efficiency hinders the effectiveness of environmental pollution control, which is mainly affected by the slow technological progress; and (3) at the provincial level, the overall efficiency of Shanghai and Guangxi has long been above 0.9, while the efficiency of other provinces has been below 0.9 for quite a long time. At the regional level, the Yangtze River Delta is the most effective area, while the Yellow River Basin is the most ineffective area. In consideration of this, we provide specific strategies for improving PCE of each province, from three aspects of increasing the capital input, optimizing the scale structure, and upgrading technology level.

- **Keywords:** Pollution control efficiency; Capital input; Three-stage global DEA; Efficiency change decomposition

Lucía Grande, Miguel Ángel Vicente, Sophia A. Korili, Antonio Gil. *Synthesis strategies of alumina from aluminum saline slags*. Pages 1010-1028.

Aluminum saline slags is a waste of the metallurgical industry that presents serious environmental problems since it needs very extensive areas for its disposal, the toxicity it causes in the atmosphere and groundwater, in addition to high transportation costs. The

valorization of this residue by the synthesis of alumina, a compound widely used in the chemical industry, generates a high impact and great interest. In this work, the strategies for synthesizing alumina from aluminum saline slags are reviewed in a context of growing demand for this metal and environmental crisis. The first sections present the aluminum production processes, both from natural bauxite (primary process) and from the recycling of materials with a high aluminum content (secondary process); paying attention to the waste generated and what environmental problems they produce. The main investigations that have allowed to address the recovery of the waste generated are described below, focusing on the processes of recovery/extraction of the aluminum present in its composition. The aluminum in these residues can be found as a metal or forming other compounds such as simple or mixed oxides. Chemical processes are the most relevant, especially those that deal with the acid and alkaline extraction of the metal. The most important section of the work reports on the methods of synthesis of Al2O3, highlighting the methods of precipitation, sol-gel, hydrothermal synthesis, and combustion, among others. The work ends with a summary and conclusions section.

- **Keywords:** Aluminum; Alumina; Saline slags; Leaching; Precipitation method; Aluminum hydroxide

Qiuhong Wang, Songling Jin, Hu Wen, Zhenmin Luo, Chi-Min Shu, Wei Gao, Liwen Wang, Xiaoyu Lu. *Dynamic characteristics of methane explosion flame propagation in three types of pipe*. Pages 1029-1047.

In process industries, the pipe connecting the various process units has complex structures. An experimental system was established to examine the flame propagation in premixed methane explosions given various methane concentrations. Three types of vented pipe, a horizontal pipe, a vertical pipe, and a T-shaped pipe, were investigated. When the methane concentration was 10 vol%, the flame propagation velocity was maximised, and the time to reach maximum flame propagation velocity (ta) was the shortest, vmax in the T-horizontal pipe was higher than that in the T-vertical pipe. The attenuation coefficient of the velocity for the vertical part was 1.16. When the methane concentration was closer to 10 vol%, the maximum flame temperature Tmax and maximum explosion pressure Pmax were higher, and the response time differences among thermocouples at different positions were more minor. The vertical bifurcation structure enabled shunting of the methane explosion shock wave and energy, and the attenuation on T and P reached up to 49.08% and 13.91%. The attenuation coefficients for the Tmax and Pmax in the vertical part were 1.50 and 1.08, respectively. The findings can provide theoretical basis for reducing and controlling the risk of pipeline accidents involving natural gas explosions.

- **Keywords:** Pipe configuration; Attenuation coefficient; Flame temperature; Explosion pressure; Vertical bifurcation structure

Sérgio M. Vilas-Boas, Débora C. do Nascimento, Rafael M. Dias, Gabriel H. Rozo, Antonio M. Barbosa Neto, Olga Ferreira, Simão P. Pinho, Mariana C. da Costa. *Flash point of binary and ternary monoterpene mixtures: Experimental and modeling*. Pages 1048-1057.

The flash point (FP) of pure or mixtures of flammable substances is an important indicator in designing fire risk mitigation and prevention measures in the chemical and oil industry. Although FP data of fuel constituents and blends are often found in the literature, studies addressing other flammable mixtures, such as essential oils (EOs) and their constituents (terpenes and terpenoids), are scarce. EOs are aromatic, volatile liquid mixtures extracted from plant matrices that present diverse biological properties and find numerous applications in the food, pharmaceutical, cosmetic, and fragrance industries. In this work, experimental FP measurements of binary and ternary mixtures of four

structurally diverse monoterpenes (carvone, eucalyptol, limonene, and linalool), widely found in different EO profiles, were carried out. Besides, the Liaw-UNIFAC model and the COSMO-RS model were used to calculate the FP data of the studied mixtures, resulting in global root-mean-square deviations (RMSD) of 2.0 K and 0.7 K, respectively. Both models deliver better predictions than the ideal approach (RMSD = 2.4 K) for the studied systems, demonstrating the importance of considering nonideal effects when estimating the FP data of terpene mixtures. These results provide essential information for accurate process safety and fire risk assessment in the EO industry.

- **Keywords:** Flash point; Monoterpene; Essential oil; Liaw-UNIFAC model; COSMO-RS; Safety

Erhui Zhang, Baokun Zhou, Lei Yang, Changfeng Li, Ping Li. *Experimental study on the microseismic response characteristics of coal and gas outbursts*. Pages 1058-1071.

A microseismic monitoring simulation experiment of coal and gas outbursts was carried out to study the microseismic response characteristics of the coal and gas outburst process. The microseismic response characteristics were analyzed from the microseismic waveform and time frequency at each stage of the outburst process. The quantitative description of the outburst process was achieved by the statistical analysis of microseismic signals and the determination of the microseismic energy index of outburst hazards. The results showed that the coal and gas outburst process included four stages: preparation, start, development, and stop, and the outburst moment is at the development stage. The protruding hole in the experiment was an ellipsoid with a small mouth and large cavity. Frequency components were complex and extensive and tended to high frequencies at the prominent stage. The frequency of the microseismic response waveform at the moment of prominence was higher than that before and after prominence, but energy at the moment of prominence was not maximum. Sudden changes in amplitudes at the preparation and development stages had more outbursts, and the maximum equivalent energy at the moment of prominence was as high as 45,000 Hz. Compared with the local high amplitude at the preparation stage, the development stage presents an overall high amplitude. Although the start stage is calmer, it is a critical period for predicting outbursts, and the microseismic activity characteristics of the outburst stage differed significantly from those of the other three stages. Quantitative indices reflecting the risk strength of coal and gas outbursts at the breeding stage were defined from microseismic energy, and the outburst risk indices under experimental conditions were established. When $L1 < 3.64$, $L2 < 0.16$, and $L3 < 5.74$, the coal mass had a weak outburst risk; when $L1 > 3.64$, $L2 > 2.33$, and $L3 > 5.74$, it had strong outburst risks. The research results provide an idea for coal and gas outburst precursor information and dynamic early warning.

- **Keywords:** Coal and gas outbursts; Microseismic; Time-frequency analysis; Quantitative description; Outburst warning

Dongjie Pang, Yanpeng Mao, Yang Jin, Zhanlong Song, Xujiang Wang, Jingwei Li, Wenlong Wang. *Review on the use of sludge in cement kilns: Mechanism, technical, and environmental evaluation*. Pages 1072-1086.

With the increasing sludge production and cement carbon emissions worldwide, there is an urgent need to develop synergistic approaches to sludge co-process in cement kilns options for building up an interactive sludge carbon reduction process. Cement kilns with temperatures as high as 1450 °C can dissipate various wastes and completely decompose or solidify harmful substances, including dioxins and heavy metals, in the cement crystal structure. Therefore, cooperative cement kiln disposal of sludge can thoroughly decompose organic components as well as their intrinsically cured heavy metals. The vast majority of cement production lines in the world are already equipped

for co-process, but the disposal of sludge is blended at a relatively small amount of about 6%. This paper first summarizes the physicochemical characteristics of different types of sludge. In addition, the discussion focuses on the sludge raw material substitution principle and the heavy metal solidification process. The mechanism of K+, Na+, and Cl- plasma damage is further investigated in depth. The overview study predicts the annual carbon emission reduction content of about 25 million tons from two routes of cement kiln co-process of sludge and other solid wastes such as raw material substitution and alternative fuels and cross industries.

- **Keywords:** Cement kiln; Sludge; Co-process; Heavy metals; Material substitution; Carbon reduction

Megan Soh, Marhaini Mostapha, Yee Ho Chai, Deni Shidqi Khaerudini, Frederick Jit Fook Phang, Jiuan Jing Chew, Soh Kheang Loh, Suzana Yusup, Jaka Sunarso. *Role of levulinic acid in catalytic wet torrefaction of oil palm trunks: Insights into the hydrochar physicochemical properties, liquid phase composition, and reaction mechanisms*. Pages 1087-1098.

This study evaluates the effects of levulinic acid addition and different operating conditions on the physicochemical and structural properties of the resultant OPT hydrochar as well as on the liquid phase composition to identify its potential reaction pathway during wet torrefaction. The addition of levulinic acid enhances the solid yield and HHV of the hydrochar and promote repolymerisation and condensation reactions for the formation of secondary char with high HHV. The highest energy yield of 66.47% was attained from the OPT hydrochar wet torrefied at 220 °C for 24 h with 1.0 M of levulinic acid. Increasing the levulinic acid concentration promoted secondary chars to agglomerate. Liquid phase analyses showed that wet torrefaction of OPT in the presence of levulinic acid promotes the hydrolysis of hemicellulose and cellulose to glucose at mild operating conditions and enhances the rehydration of 5-HMF to levulinic acid.

- **Keywords:** Hydrothermal carbonisation; Oil palm biomass; Organic acid catalyst; Reaction pathways; 5-hydroxymethylfurfural (5-HMF)

Fei He, Baozhong Ma, Chengyan Wang, Yongqiang Chen, Xiujuan Hu. *Surfactant-enhanced extraction of valuable metals from limonitic laterite: Porous kinetics and mechanism analysis*. Pages 1099-1109.

The efficient extraction of valuable metals from low-grade mineral resources is an important initiative to implement the concept of carbon neutrality and achieve energy conservation and emission reduction. Atmospheric leaching of laterite ores is widely noted for its low cost. However, low extraction and difficulties in slurry filtration have severely restricted its development. Inspired by our previous studies on the porous kinetics, two options for improving the nitric acid atmospheric leaching (NAAL) of limonitic laterite are proposed. 84.85 % of Ni extraction is achieved under the optimal process conditions (Temperature: 98 °C, Time: 3.5 h, Liquid/Solid: 4.7 mL/g, and the initial nitric acid concentration: 487 g/L). After enhanced treatment, the Ni extraction is increased by 3.16 % (bleed air), 4.55 % (SDS: sodium dodecyl sulphate), and 5.67 % (DTAB: dodecyl trimethyl ammonium bromide), respectively. In addition, DTAB not only promotes the leaching of laterite ores but also improves the filtration performance of the slurry. The filtration rate was more than three times higher than in the absence of DTAB. The presence of silicic acid is responsible for the difficult filtration of the slurry and the low extraction of valuable metals. Analysis of the intensification mechanism shows that the bleed air treatment mainly eliminates the obstruction of leaching by air in the pores, thus increasing the effective reaction area. The reinforcing effect of surfactants is mainly due to the improvement of diffusion efficiency, the reduction of adsorption, and the

increase in permeability. This paper provided a feasible option for the enhanced leaching of limonitic laterite, and the reinforcement mechanism was explained clearly. It not only responds to the call for energy conservation and emission reduction by achieving efficient extraction of valuable metals from low grade laterite resources, but also avoids the treatment of laterite ores by means of high temperature and pressure.

- **Keywords:** Surfactants; Extraction; Limonitic laterite; Enhancement; NAAL; Ni

Jia Liu, Liang Tang, Yaqing Liu, Dan Zhang, Xinshu Jiang. *Insights into characterization of organophosphorus flame retardants transformation under thermal activation persulphate*. Pages 1110-1119.

Organophosphorus flame retardants (OPFRs) are widely used in consumer products and are frequently detected in water, thereby threatening public health. In the present study, we investigated the mechanism of degradation of two representative OPFRs, tri(2-chloroethyl) phosphate (TCEP) and tri-n-butyl phosphate (TnBP), by thermally activated persulphate (PS). First, the experimental data were in accordance with the modelling simulations. In the absence of Cl−, the instantaneous concentration of SO4−• was 3.12 × 10−15 M. When the concentration of Cl− increased from 7.5 mM to 450 mM, Cl2−• became the dominant radical, with its concentration increasing from 7.39 × 10−14 M to 7.91 × 10−13 M. Conversely, the concentration of SO4−• declined from 6.3 × 10−17 M to 2.6 × 10−19 M. Second, owing to the transition of dominant radicals from SO4−• to Cl2−•, the resultant pseudo-first-order decay rates (robs) of TCEP and TnBP were reduced. Without Cl−, robs of TCEP and TnBP were (1.8 ± 0.1)× 10−2 h−1 and (6.1 ± 0.4)× 10−2 h−1, respectively. When the Cl− concentration reached 450 mM, the robs of TCEP and TnBP dropped to (2.2 ± 0.2)× 10−3 h−1 and (2.4 ± 0.2)× 10−2 h−1, respectively. Additionally, despite the presence of oxidised Cl2−• compounds, when Cl− participated in PS oxidation, no primary organic chlorinated byproducts were detected. These results indicated that Cl− did not affect the toxicity of TCEP and TnBP transformation intermediates. Finally, the apparent kinetic isotope effects for carbon (AKIEC) and hydrogen (AKIEH) were detected to be 1.01 and 1.370–3.049, respectively. The results implied that the C-H split occurred during the PS-activated transformation of TCEP and TnBP. The present study combines quantitative steady-state radical calculation, transformation product identification, and isotope fractionation to characterise the radical transformation of typical OPFRs, thereby laying the foundation for regulating PS oxidation to eliminate OPFRs in real-world systems.

- **Keywords:** OPFR; Steady-state radical modelling; Transformation product; Toxicity; Isotope fractionation

Ana Pilar Melendo, Roberto Berbés, Sofía T. Blanco, Javier Fernández. *Effect of the impurities O2 or NO present in non-purified flue gas from oxy-fuel combustion processes for carbon capture and storage technology*. Pages 1120-1131.

CO2/impurities cocapture in CCS technology allows reducing the purification costs and avoiding the emission of pollutants into the atmosphere. The viability of the transport by pipeline and the geological storage of the non-purified flue gas from oxy-fuel combustion of biomass and other processes, keeping the impurities O2 or NO in the stream along with CO2, is assessed considering thermodynamic and hydraulic aspects. For this, we experimentally determined, under CCS conditions, the density, vapor-liquid equilibrium, and speed of sound of three CO2 + O2 and CO2 + NO mixtures as binary models of the gas, and we calculated their Joule-Thomson coefficients from the experimental data. Additionally, we compared the values calculated for the determined properties using the equations of state EOS-CG, GERG-2008 and PC-SAFT to our results of CO2 + O2, validating all three equations for this system. For the CO2 + NO mixtures, only PC-SAFT

could be applied, which was also validated using the parameters obtained in this work. Finally, we calculated several selected CCS parameters from our data and concluded that both O2 and NO have negative effects on the transport and storage steps of this technology, which are negligible in the case of NO with the investigated concentrations.

- **Keywords:** CCS; Carbon dioxide; Nitric oxide; Oxycombustion; Thermodynamic properties; Equations of state

Ding Jiang, Hongping Li, Xiaoxue Cheng, Qifan Ling, Hao Chen, Bahram Barati, Quanfeng Yao, Abdelfatah Abomohra, Xun Hu, Pietro Bartocci, Shuang Wang. *A mechanism study of methylene blue adsorption on seaweed biomass derived carbon: From macroscopic to microscopic scale*. Pages 1132-1143.

Biomass based active adsorbent can be prepared by activation process to adsorb dyes. In this study, using macroalgae as raw material, the biomass based activated carbon material was prepared by NaOH activation method to adsorb methylene blue. The activated adsorbent with high specific surface area (1238.491 m2 g−1) was characterized by BET, XRD, FTIR and XPS. The effects of impregnation ratio, amount of adsorbent, pH and contact time on the adsorption activity of biochar on MB were evaluated. The adsorption kinetics, molecular dynamics and density functional theory were discussed. The maximum MB removal efficiency of SWAC reached 98.56 % at 30 °C and pH= 5 which is due to its large specific surface area and mesoporous slit structure. MD simulation shows that MB molecules were adsorbed on carbon layer through face-to-face stacking. DFT calculation and subsequent electron structure analysis suggested that a synergistic effect of π-π stacking, cation-π interaction, and electrostatic interaction could help stabilize adsorbed MB molecules. And an excellent adsorption capacity SWAC is due to its graphitic N sites for high electronegativity.

- **Keywords:** Seaweed; Adsorption; Dye; Molecular dynamics; Density functional theory; Biochar