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Daniele Di Trapani, Federica De Marines, Pietro Greco Lucchina, Gaspare Viviani. *Surfactant-enhanced mobilization of hydrocarbons from soil: Comparison between anionic and nonionic surfactants in terms of remediation efficiency and residual phytotoxicity*. Pages 1-9.

The aim of the present study was to assess the effectiveness of two surfactants (Polysorbate 80 – Tween 80 and Sodium Dodecyl Benzensulphonate – SDBS) for the remediation of hydrocarbon-contaminated soil. To study the effectiveness of these surfactants, an experimental laboratory-scale apparatus was set up for the simulation of a soil flushing intervention. Different surfactant concentrations and flushing flow rates were investigated. At the end of the experiments, the removal efficiency was evaluated and phytotoxicity tests were performed by means of germination index (GI). Results showed that the use of both surfactants allows to reach high removal efficiency (~50% for Tween 80 and ~70% for SDBS) of hydrocarbons from soil and that either the surfactant concentration and the contact time between surfactant and contaminant affected the extraction performance. GI results showed different effects of the two surfactants on the phytotoxic features of the soil after treatment. Indeed, while the soil treated with SDBS was found to be more phytotoxic, leading to a lowering of the GI (10.88 %), the soil samples flushed with Tween 80 were characterized by higher values (146.61%). These results might be of interest in the case of surfactant application in remediation interventions in soils intended for future agricultural activity.

- **Keywords:** Soil flushing; Soil remediation; TPH; Surfactants; SEAR; Phytotoxicity

Majid Bagheri, Nakisa Farshforoush, Karim Bagheri, Ali Irani Shemirani. *Applications of artificial intelligence technologies in water environments: From basic techniques to novel tiny machine learning systems*. Pages 10-22.

Artificial intelligence (AI) and machine learning (ML) are novel techniques to detect hidden patterns in environmental data. Despite their capabilities, these novel technologies have not been seriously used for real-world problems, such as real-time environmental monitoring. This survey established a framework to advance the novel

applications of AI and ML techniques such as Tiny Machine Learning (TinyML) in water environments. The survey covered deep learning models and their advantages over classical ML models. The deep learning algorithms are the heart of TinyML models and are of paramount importance for practical uses in water environments. This survey highlighted the capabilities and discussed the possible applications of the TinyML models in water environments. This study indicated that the TinyML models on microcontrollers are useful for a number of cutting-edge problems in water environments, especially for monitoring purposes. The TinyML models on microcontrollers allow for in situ real-time environmental monitoring without transferring data to the cloud. It is concluded that monitoring systems based on TinyML models offer cheap tools to autonomously track pollutants in water and can replace traditional monitoring methods.

- **Keywords:** Artificial intelligence; Deep learning; TinyML; Microcontrollers; Monitoring

Qiyong Zhou, Weitong Ma, Hui Shi, Song Lu, Heping Zhang. *Enhancement and suppression of counterflow diffusion flame by HFC-125*. Pages 23-34.

Efficient fire extinguishing is a safety prerequisite for protecting the environment from fire damage. Understanding the effect of fire extinguishing agent on flame in complex environment is basic work for efficient fire extinguishing. We investigate the impact of HFC-125 on the extinguishment of propane-air highly stretched diffusion flames. Flame thickness is measured using the proportional method. Parameters such as dimensionless flame stand-off distance and flame stretch rate are calculated. Low concentrations of HFC-125 initially increase the flame thickness, but as the concentration increases further, the flame thickness decreases and the flame suppression effect of HFC-125 intensifies. HFC-125 reduces the amount of carbon soot generated and accelerates the transition from yellow to blue flame. Within a specific concentration range, N2 has a minimal effect on flame structural parameters compared to HFC-125. High concentration of N2 forms a high bright blue flame, while HFC-125 reacts with the flame to form a blue-violet flame. Compared to HFC-125, HFC-227ea can significantly reduce flame thickness and increase dimensionless flame stand-off distance, exhibiting a notable suppression effect. Furthermore, high concentrations of HFC-125 substantially reduce the critical flame stretch rate and provide a lower extinguishing concentration in counterflow diffusion flames than in the cup burner.

- **Keywords:** HFC-125; Fire suppression; Counterflow diffusion flame; Extinguishment

Hao Ren, Xiaojun Liang, Chunhua Yang, Zhiwen Chen, Weihua Gui. *Spatial-temporal associations representation and application for process monitoring using graph convolution neural network*. Pages 35-47.

Modern industrial processes generate many dynamic, associated, and multi-scale variables, which are more likely to implicit spatial-temporal associations knowledge for describing irregular changes at different times. Inspired by this, a novel spatial-temporal associations representation method is proposed for process monitoring. Specifically, numerous variables and their associations simultaneously can be utilized to construct a static graph network snapshot. Then, graph network snapshots corresponding to process states at different times are fed into a graph convolutional neural network to implement graph classification. Finally, process monitoring is realized by continuously identifying each snapshot. Monitoring feasibility and applicability are demonstrated by the Tennessee Eastman (TE) benchmark and cobalt removal process application.

- **Keywords:** Spatial-temporal Associations Representation; Process Monitoring; Graph Network Snapshot; Graph Convolutional Neural Network

Do-Gyun Kim, Sarah Witherrite, Liang Yu, Quanbao Zhao, Shulin Chen. *Novel ammonia recovery from anaerobic digestion by integrating biogas stripping and gypsum absorption*. Pages 48-55.

Recovering ammonia from anaerobic digestion (AD) effluent offers the opportunity to produce a renewable fertilizer and reduce environmental impact. A novel process developed for such an application was evaluated during this study. The feature of the process is integrating biogas stripping and gypsum (CaSO4·2H2O) absorption. The result revealed that the lower CO2 content and the absorption temperature contributed the higher efficiency of ammonia recovery. The gypsum solution recovered around 95% of the stripped ammonia when the stripping gas contained 10% CO2 and it rose to 100% when the gas contained more than 30% CO2. Furthermore, a statistical model and genetic algorithm were applied to estimate the total ammonia recovery and optimize the operating parameters. The experimental and modeling results indicated that integrating biogas stripping with gypsum absorption can effectively harvest ammonia nitrogen and reduce CO2 emissions while producing (NH4)2SO4 fertilizer from AD effluent.

- **Keywords:** Biogas stripping; Gypsum absorption; Multiple regression; Genetic algorithm

Zhen Shen, Yu Liu, Junhuan Lei, Weijun Shen, Yuheng Wang, Cheng Xu, Jiaxun Gong. *Changes in the three-dimensional molecular structure of coal during methane adsorption induced swelling*. Pages 56-66.

Methane (CH4) adsorption-induced swelling is one of the critical factors controlling the permeability of coalbed methane (CBM). CH4 adsorption alters the molecular structure of coal so as to induce coal swelling, and many uncertainties still exist in the process. In this study, the change in the molecular structures of different chemical structures by CH4 adsorption was investigated using the Grand Canonical Monte Carlo method to simulate the alteration of bond lengths and bond angles during swelling. The results demonstrate that the alteration of chemical structure is more extensive than a chemical bond, which is the critical factor causing the swelling behavior. Owing to the complex molecular structure of coal, among the different types of chemical structures, the C-O-C (-O-) chemical structure showed the most significant change in bond angle, with the largest degree of change is 12.89%. Compared with other chemical structures, the C-C-C (aromatic -C-) chemical structures are more stable and the largest degree of change is 0.65%. For the different types of chemical bonds, the C-C chemical bonds showed the most significant change in bond lengths, with the largest degree of change is 2.94%. And the O-H chemical bond showed the smallest change, with the largest degree of change is 0.79%. Considering the structure evolution of coal, the C-O-C (-O-) chemical structure decreases with increasing maturity and changes to the greatest after the adsorption of methane. The aromatic structure increases and the degree of deformation decreases, which is consistent with the previous experimental values for swelling. These results reveal the details of different types of chemical group deformation, providing a molecular-level insight into adsorption swelling and permeability changes.

- **Keywords:** Methane adsorption; Chemical structure; Chemical bond; Coal macromolecular structure

Hongmei He, Xiaohui Sun, Li Ma, Hadi Ghaebi. *Development of a new multi-generation system integrated with the S-Graz and Cu-Cle cycles for ammonia, hydrogen and power generation*. Pages 67-77.

A new multi-generation plant incorporated with the ammonia synthesis reactor, a Cu-Cl cycle, and a S-Graz cycle plus a gas turbine cycle for electricity, hydrogen as well as ammonia production recommended and dissected from exergy, energy, exergoeconomic,

exego-environmental, and environmental (5E) aspects, in this research. Furthermore, to investigate the effect of input variables on the plant function criteria, exhaustive sensitivity evaluations were carried out and disputed in detail. The exergy and energy yields, the products 'sum unit cost, the cost rate of environmental penalty as well as the emission rate of the offered poly-generation plant have been 41.16%, 45.57%, 369.6 $/GJ, and 0.0001319, respectively. Besides, the plant provided the net power output, hydrogen, and, ammonia of 151488 kW, 0.2199 kg/s, and 1.884 kg/s, sequentially. Also, the whole exergy destruction rate of the plant was computed at about 128.289 MW. Finally, the sensitivity investigations resulted that increasing the hydrogen molar flow rate and high-temperature turbine (HTT) inlet temperature had a positive effect on the techno-eco-environmental performances of the system.

- **Keywords:** Exergoenvironmental analysis; Hydrogen production; Ammonia synthesis; S-graze cycle; Techno-economic-environmental analyses; Power production

S. Miralles-Cuevas, R. Salazar-González, A. Cabrera-Reina. *Exploring the scalability of solar-activated persulfate with iron-EDDS in raceway pond reactors for advanced wastewater treatment*. Pages 78-88.

In this study, the removal of microcontaminants (MCs) by the activation of persulfate (PS) with Fe(III)-EDDS under natural solar radiation in a low-cost raceway pond reactor (RPR) was investigated. The primary focus was to evaluate the effect of the Fe(III)-EDDS molar ratio, initial iron concentration, PS concentration, and initial pH on process performance while using sulfamethoxazole (SMX) and carbamazepine (CBZ) as model MCs. The investigation encompassed three different water matrices: natural water, synthetic municipal wastewater treatment plant (MWWTP) secondary effluent, and actual MWWTP secondary effluent. During experiments in natural water, it was found that 0.1 mM Fe(III) at a 1:2 molar ratio and 0.2 mM Fe(III) at a 1:1 molar ratio resulted in the most adequate operational conditions. Further experiments revealed a general decrease in process efficiency due to water matrix effects; however, this could be compensated by increasing the initial PS concentration and decreasing the initial operation pH. For example, the use of 0.2 mM Fe(III) at a 1:1 Fe(III):EDDS molar ratio, with 2 mM PS at pH 6, allowed for an 80% removal of the MCs sum in approximately 20 min, along with a significant decrease in chronic toxicity (Selenatrum Capricornutum) when working with actual waters. Nonetheless, the final experiment, focused on simultaneous MCs removal and wild bacteria inactivation in actual MWWTP secondary effluent, showed only a 1.6–1.8 log reduction of Escherichia coli, total coliforms, and Enterococcus faecalis. As such, further studies about the solar/Fe(III)-EDDS/PS process are needed to explore new strategies that improve its disinfection efficiency.

- **Keywords:** Microcontaminants; Wastewater treatment; Chronic toxicity; Persulfate; Sulfate radical, disinfection

Bhanu pratap pulla, Tirumala Uday Kumar Nutakki, Aliashim Albani, Manoj Kumar Agrawal, M.Yasmin Begum, Wenju Han. *Comprehensive technical study of a novel polygeneration arrangement using natural gas power plant and geothermal energy for producing electricity, heat, fresh water, and methanol*. Pages 98-121.

Structural modifications play a crucial role in enhancing the sustainability of natural gas power plants owing to their significant contribution to greenhouse gas emissions and irreversibility factors. One primary solution is using waste heat recovery systems integrated with these power plants, producing different products. Furthermore, integrating renewable energy resources into the entire system within a co-feed framework may be a viable method for further enhancements. The current study focuses

on a novel heat integration process combined with a natural gas power plant, which uses geothermal energy as an auxiliary energy source. The newly designed system encompasses a gas turbine cycle, two modified geothermal power plants, a water electrolyzer unit, and a methanol synthesis unit. The process is simulated utilizing the Aspen HYSYS software, and to evaluate its viability, analyses are performed pertaining to energy, exergy, environment, and economics. Furthermore, a comprehensive parametric analysis is conducted on the primary performance indicators. The simulation results show that the process's energy, exergy, and electrical efficiencies equal 53.85%, 47.30%, and 40.26%, respectively. The environmental evaluation demonstrates that the specific carbon dioxide emissions associated with the total energy produced and the sum of power and heating are 0.27 kg/kWh and 0.294 kg/kWh, respectively. From the economic aspect, the total unit cost of the products and the cost of energy of the system are 20.69 $/GJ and 0.086 $/kWh, respectively. Also, total annual cost, investment cost, and net present value of 222.81 M$, 1010.64 M$, and 1220.57 M$, respectively.

- **Keywords:** Polygeneration arrangement; Geothermal power plant; Methanol synthesis; Aspen HYSYS; Economic analysis; Low CO2 emission

Sampath Suranjan Salins, Shiva Kumar, Jatin Chouhan, Ana Tejero-González, Prashant Sreekumaran Nair. *Experimental performance of a spray tower system for water desalination and indoor thermal comfort*. Pages 122-135.

Present work characterizes a spray tower-based desalination system, designed to simultaneously provide fresh water by condensation and supply dehumidified air to occupied spaces. Its configuration is open air-open water, with Celdek 7090 packing in the humidification section and water-cooled helical coils for dehumidification. The performance parameters calculated are: gained output ratio, recovery ratio, coefficient of performance, specific electrical energy consumption, mass ratio, humidification, and dehumidification efficiency. This performance is analyzed for varying air Reynold's number and water flow rate. The best results were obtained for the sea water flow rate tested of 18 liters per hour, and showed maximum humidification efficiency, dehumidification efficiency, COP, freshwater rate, gained output ratio and concentration factor equal to 87.14%, 94.56%, 3.34, 0.9 liters per hour and 1.05, respectively. Exit air meets the thermal comfort requirements which avoids the ventilation thermal loads in the space cooling.

- **Keywords:** Desalination; Humidification; Dehumidification; Predicted mean vote; Thermal comfort

Jingyu Zhao, Xiaocheng Yang, Jiajia Song, Yongli Zhang, Chi-Min Shu. *Experimental study of coal spontaneous combustion high-temperature region spreading characteristics*. Pages 136-147.

To solve the difficult problem of determining the change law of key point temperature and gas during the motion of high temperature area inside the coal mine seam, this study used the simulation platform of coal spontaneous combustion (CSC) development to investigate the temperature, gas concentration, functional group migration, and change rule of key points with layers in the holistic process of high-temperature region (HTR) spreading of Wen-Zhuang coalmine in Shanxi province, China. The analysis involved the dynamic change rule among temperature, oxygen consumption rate, CO, and C2H4. Finally, with the gray correlation method, the changes of the dominant functional groups released by CO and C2H4 were explored, which revealed the transport rule between the functional groups and the regional spreading in the HTR spreading process. The results show that the temperature of coal body and the rate of oxygen consumption gradually decreased with the deepening of coal layers. Among them, as the

coal seam burns, the coal body will appear to "collapse", along with the phenomenon of "re-ignition"; at the combustion point temperature of each coal layer, the activity of the oxygen-containing functional group was the largest, the activity of hydroxyl group was the smallest, and the activity of aliphatic and aromatic hydrocarbons was similar. Among them, the hydroxyl group, aromatic hydrocarbon, and oxygen-containing functional group had the same trend changing with the deepening of the layers, exhibiting a trend of first decreasing after increasing and later decreasing, and positively correlated with the ignition temperature of each layer. The trend of aliphatic hydrocarbon was opposite to the trend of other functional groups and negatively correlated with the ignition temperature of each layer. The research results of this paper can be used for disaster prevention in the HTR of mine fires, and parameters, such as indicator gases, functional groups and temperature, can be used to determine and deter the migration trend of mine fires, providing a theoretical basis for the prevention and control of high-temperature diffusion of coal spontaneous combustion.

- **Keywords:** Functional group migration; Oxygen consumption rate; Gray correlation method; Transport rule; Ignition temperature

Zezheng Lin, Yang Guo, Xiaoxuan Qu, Yuying Xiang, Shuwen Shen, Xin Zhu. *Degradation of bisphenol A by Fe-doped BiOBr enhanced UV/persulfate system: Significant role of superoxide radicals*. Pages 148-159.

Widely diffused pollution of endocrine disrupting chemicals (EDCs) has indeed threatened the safety of ecological environment and human health. A hydrangea-like Fe doped BiOBr (Fe-BiOBr) microsphere was synthesized and used to enhance the performance of UV/persulfate (PS) system using bisphenol A (BPA) as the targeted contaminant. The photochemical characterization of Fe-BiOBr showed that Fe doping markedly improved the separation efficiency of photoelectron and hole, and enhanced the utility rate of luminous energy of BiOBr. Degradation test demonstrated that with the assistance of Fe-BiOBr, the efficiency of UV/PS system was increased by 1.8 times, while 85.7% of BPA can be degraded within 10 min. Through scavenging experiments, sulfate radical (SO4•−), superoxide radical (O2•−), and hole were demonstrated as the dominate reactive species (RSs) in UV/Fe-BiOBr/PS system. Then, the role and mutual transformation of RSs was further clarified by radicals steady-state concentrations estimation and X-ray photoelectron spectroscopy (XPS) analysis. Based on the results, the produced O2•− can be subdivided into confined O2•− and free O2•− from the UV induced oxygen vacancy and photoelectron, respectively. Of which, SO4•− and confined O2•− were symbiotic via the redox cycle of Fe species. Significantly, only 2.6% of TOC can be simultaneously removed within 10 min treatment time, suggesting the incomplete degradation of BPA. For this, 16 organics was detected using LC-MS and the degradation route of BPA was also determined based on the intermediates analysis. Finally, the application possibility of the system was evaluated from the perspective of ecotoxicity by ECOSAR and T.E.S.T. softwares. This study investigates the dual effect of transition metal doped semiconductor on coupling system, and provides new insights into the role of O2•−.

- **Keywords:** Bismuth oxybromide; UV/persulfate; Bisphenol A; Superoxide radicals

Peng Xu, Zhuoyu Yang, Pengfei Zhu, Xin Liu, Ruoxi Wu, Baolin Hou. *Combination of zero-valent copper and ferric ion promoted the activation of hydrogen peroxide: Deep insight into interaction mechanism and reactive species*. Pages 160-168.

Zero-valent copper (ZVC) activated hydrogen peroxide (H2O2) was widely used to degrade various organic pollutants due to its excellent degradation performance.

However, under acidic condition, the low efficiency inhibited the pollutants degradation efficiency. In this study, the supplement of ferric ion (Fe(III)) markedly improved the orange G degradation in the ZVC/H2O2 system. Various reactive species such as hydroxyl radical (•OH) and Fe(Ⅳ) were identified, besides the contribution rate of the reactive species could be adjusted by changing the reaction parameters. During the degradation of orange G, ZVC furnished Cu(I) by hydrogen erosion and the reaction with O2 and H2O2, and then ZVC and Cu(I) boosted Fe(III)/Fe(II) circulation, part of Fe(II) and Cu(I) activated H2O2 to generate •OH, another part of Fe(II) reacted with H2O2 to generate Fe(Ⅳ), resulting in orange G removal. Common coexisting substances in natural water bodies such as nitrate ion and sulfate ion hardly influence the removal of orange G, while Cl- notably enhanced the removal of orange G, and humic acid markedly suppressed the decoloration of orange G. Orange G removal by the ZVC/Fe(III)/H2O2 system showed outstanding performance in actual water samples. In addition, the total dissolved copper complied with the II-level environmental quality criteria after alkali precipitation. All the above facts bespoke the ZVC/Fe(III)/H2O2 system had substantial application prospects.

- **Keywords:** Fe(IV); •OH; ZVC/Fe(III)/H2O2 system; Fe(III)/Fe(II) cycle; Orange G

Xue-ying Yuan, Xin-yue Zhao, Ying-zhou Chen, Zhi-shan Yang, Jin-yan Yang. *Stabilization effect of chelating agents on heavy metals in two types of municipal solid waste incineration fly ash*. Pages 169-180.

Municipal solid waste incineration (MSWI) fly ash is complex in composition and contains large amounts of heavy metals. To investigate the effects of different passivating agents on Cd, Pb, Cr, Ni and Zn in different types of fly ash, 7 reagents were selected as passivating agents, including 3 inorganic reagents (Na2S, Na3PO4, NaH2PO4) and 4 organic reagents (SDD, DDTC, TMT, thiourea). The results showed that at low addition levels, sulfur-containing organic chemicals and phosphates were more effective in chelating these metals in both grate furnace incineration fly ash (GF FA) and circulating fluidised bed incineration fly ash (CFB FA), while Na2S was more effective in chelating heavy metals in CFB FA. In addition, agents containing -N-CS groups showed better chelation of heavy metals in GF FA, while heavy metals in CFB FA were more affinity to agents containing -SH groups. The ternary compound TMT-NaH2PO4-SDD (m1:m2:m3 = 2:3:1) was an excellent chelating agent for Pb, Cd in the GF FA, and TMT-Na2S-thiourea (m1:m2:m3 = 2:1:3) was a suitable chelating agent for these metals in CFB FA. The chelation rate of Cd and Pb after the treatments mixed ternary reagents was above 99%, and the leaching amount was much lower than the limit value of pollution control standards for domestic landfills. Moreover, under different pH leaching conditions, the leaching concentrations of Cd and Pb in the fly ashes treated with the ternary mixture were lower than the standard limits. In general, the ternary compound can effectively chelate heavy metals in fly ash, which provides a reference for selecting a suitable stabilizer combination for heavy metal in fly ash.

- **Keywords:** Stabilization/solidification (S/S); Fly ash; Heavy metals; Chemical chelating agent

Gholamreza Goudarzi, Zeynab Baboli, Jafar Fatahiasl, Yaser Tahmasebi Birgani, Zeinab Ghaedrahmat, Golnaz Masiri, Mahdis Goudarzi, Negin Bashirian. *On the concentration of radon in a polluted city of the Middle East: An insight into its association with PM levels, air properties, and risk assessment*. Pages 181-191.

This study was conducted in Ahvaz city, where the concentrations of radon and airborne particles in 10, 2.5, and 1 micrometers, along with meteorological parameters were

measured. The measurements were performed in three educational and therapeutic sampling points at both ground and underground levels during cold and hot seasons. The results showed that in 3.17% of the samples, the concentration of radon exceeded the permissible limit recommended by the Environmental Protection Agency (EPA). Factors affecting the increase of radon concentration in indoor air included cold season, underground sampling points, the number of doors and windows as air dilution factor and air exchange, air pressure, and air humidity. The concentration of particles in the air did not have any effect on radon in the indoor air. The annual effective dose of exposure to radon (DR), the annual effective dose of lung (DE), and the risk of lung cancer cases (LCC) during both cold and hot seasons and at ground and underground levels were lower than the permissible values recommended by the International Committee on Radiological Protection (ICRP). We concluded that the increase of particles is neither the cause nor the source of increased indoor air radon. The findings of the present investigation recommend controlling physical indoor air parameters particularly temperature and relative humidity by proper ventilation systems to mitigate the impact of radon exposure on inhabitants.

- **Keywords:** Radon concentration; Particle concentration; Meteorological parameters; Risk assessment; Ahvaz

Zibin Pan, Qingqiang Gao, Zuliang Chen. *Removal of As(Ⅲ) and As(Ⅴ) from mine groundwater using bimetallic Fe/Cu nanoparticles*. Pages 192-204.

The elimination of arsenic (As) from arsenic-contaminated mine groundwater has become a worldwide problem because it causes environmental degradation and poses serious risks to human health. In this study, biosynthesized Fe/Cu nanoparticles (Fe/Cu NPs) were used for the simultaneous elimination of As(Ⅲ) and As(Ⅴ) from aqueous solution, resulting in their maximum amounts removed at 8.5 and 17.5 mg/g, respectively. SEM, FTIR, and XPS characterizations indicate that the Fe component on the Fe/Cu NPs acted as an adsorption and catalyst, while the Cu component mainly developed into a co-precipitation reaction with the As species, also facilitating the Fe catalytic processed. Meanwhile, adsorption isotherms, kinetics, and DFT calculations reveal that the removal of As(Ⅲ) was primarily physical/chemical adsorption and oxidation, while the elimination of As(Ⅴ) was co-precipitation and chemisorption. The most stable adsorption site, receiving 0.252 and 0.306 electrons from As(Ⅲ) and As(Ⅴ), respectively, was the unsaturated complexes of iron on the Fe/Cu NPs. Finally, the measurements and XPS results of Fe/Cu NPs in the treatment of groundwater show that the reduced capacity to remove As was attributed to a complex reaction system that disrupted the function of the Cu component, including co-precipitation and made the catalytic process possible. This explains there are differences in the reaction processes of biosynthetic Cu/Fe NPs in aqueous solution and groundwater.

- **Keywords:** As(Ⅲ)/As(Ⅴ); Fe/Cu NPs; Mine groundwater; Removal mechanism

H.M. Reijonen, W.R. Alexander, S. Norris. *Resilience in knowledge management – the case of natural analogues in radioactive waste management*. Pages 205-222.

In the field of radioactive waste management, particularly the geological disposal of higher activity radioactive waste, support for the longevity of engineering solutions in the repository is partly based on studies of natural systems, especially geological examples, often referred to as natural analogues (NA). Since the radioactive waste can be hazardous over hundreds of thousands of years, the long-term safety has to be assessed to very far future, e.g. up to 1 Ma from now. NA studies cover and exceed the time spans of interest. Despite of the long-acknowledged importance of NAs in the safety case for

the geological disposal of radioactive waste, there is a lack of guidance and strategic planning to incorporate this information to the safety cases that assess the overall safety of the repositories – this leads to a certain lack of resilience. This paper presents the work undertaken to develop a strategy for utilising natural analogues (NAs) in Nuclear Waste Services (NWS), UK, geological disposal facility (GDF) programme. The work is largely based on the extensive review of the strategic use of NAs in the international context, lessons learnt from various past programmes and by considering how the strategy could look like in the current framework of the UK's GDF programme. The strategy presented aims to support this programme. The main message is that NA information and projects can and should be handled through the same procedures as any research utilising existing and upcoming NWS protocols. This means that NAs need to be a part of knowledge management, rather than, for example, a stagnant database. Including NAs as part of the data screening allows the knowledge base to be updated according to needs arising from the changes in the GDF programme when moving from generic stage towards more site and design specific phases. It is foreseen that key to the best utilisation of NA information is to include it in the NWS' digital safety case, making the information and the related methodology transparent. This paper refers to NWS' GDF siting programme as at September 2023.

- **Keywords:** Natural analogues; Geological disposal; Waste disposal; Radioactive waste; Nuclear waste; Risk assessment; Long-term safety; Knowledge management

Li-Hua Wen, Hong-Yao Liu, Dariush Heydarian. *Multi-objective grey wolf optimization of four different geothermal flash -organic Rankine power cycles*. Pages 223-241.

Geothermal energy, a sustainable and abundant resource, has garnered significant attention for its potential to contribute to the world's growing energy demands. Integrating organic Rankine cycles with geothermal flash cycles has emerged as a promising avenue in this pursuit. Four feasible arrangements are proposed, and their productivity and thermodynamic/economic criteria are compared. The four processes include a single flash-single loop, a dual flash-single loop, a single flash-dual loop, and a dual flash-dual loop. These structures are optimized in four scenarios: energetic efficiency/net output electrical power, energetic efficiency/payback period, exergetic efficiency/net output electrical power, and exergetic efficiency/payback period. The optimization results show that a dual flash–dual loop brings out the optimum productivity compared to the other arranged structures. The dual flash–dual loop configuration consistently outperforms the others, emerging as the optimal solution for maximizing productivity while ensuring economic viability in geothermal energy utilization via organic Rankine cycles. In conclusion, this study not only advances understanding of the synergistic potential between organic Rankine cycles and geothermal flash cycles but also provides invaluable guidance for stakeholders seeking to harness the full potential of geothermal energy with a keen eye on efficiency, sustainability, and economic feasibility.

- **Keywords:** Geothermal flash cycle; Organic Rankine cycle; Zeotropic mixture; Comparative study; Thermodynamic/economic criteria; Multi-objective optimization

Zhi Huang, Jiang Yu, Xiao Shao, Yinying Jiang, Jie Yu, Siwei Deng, Peirou Li. *Interpretable artificial intelligence for advanced oxidation systems: Principle, operations and performance*. Pages 242-259.

Advanced oxidation processes have been widely studied and employed due to their potent mineralization capacity for pollutants. However, the intricate reaction mechanisms of these processes pose limitations for fitting and predicting performance. In this study, we comprehensively derived and assessed neural networks for three advanced oxidation

methods: catalytic oxidation, catalytic wet air oxidation, and electrochemical oxidation. Our analysis encompassed multilayer perceptron principles, forward and back propagation process, strategies for handling overfitting, and performance evaluation matrices. Additionally, we utilized Bayesian optimization to probe the impact of network architecture on outcomes. Two conventional methods, multiple linear regression and response surface methodology, are employed for comparison. Our results demonstrate that neural networks exhibit more robust performance in fitting and predicting advanced oxidation processes as indicated by statistical indicators. Importantly, we tackle the "black box" issue of neural networks by incorporating the shapley additive explanations interpretable model of game theory to elucidate the impact of advanced oxidation features on outcomes. The superior performance of explainable artificial intelligence techniques implies their vast potential for broad applications in environmental science and technology.

- **Keywords:** Advanced oxidation process; Artificial intelligence; Principles; Operation; Shapley additive explanations

Chen Liu, Shoujun Zhou, Yaling Zhang, Chi Zhang, Xiangrui Liu. *Leakage diagnosis of district heating-network based on system simulation and PCA_BP neural network*. Pages 260-273.

To increase leakage diagnosis (LD) efficiency of heating-networks and overcome the lack of actual leakage data, a LD method is proposed based on system simulation and principal component analysis (PCA)_back propagation (BP) neural network that treats the LD problem as a pattern recognition one. In this method, a hydraulic working-condition (HWC) simulation model is constructed to obtain model datasets (MD) of heating-network operation and HWC experiments are conducted to obtain experimental datasets (ED), then cross datasets (CD) is constructed by mixing MD and ED with different ratio. These three datasets are handled through the PCA to unify data feature distribution and realize feature transfer learning in neural network. Then two BP neural networks are trained by ED and CD respectively and both tested with ED. Finally, four kinds of experimental heating-networks, including a branch network with single heat source (B-SHS), a branch network with double heat sources (B-DHS), a single-ring network with single heat source (SR-SHS) and a double-ring network with double heat sources (DR-DHS), are researched. The results indicate that the LD prediction accuracy of BP neural network trained by CD is higher than that one trained by ED. The LD prediction accuracy varies with the cross-data ratio: from 97.52% to 92.21% for B-SHS, from 97.23% to 92.02% for B-DHS, from 97.85% to 89.74% for SR-SHS, and from 95.89% to 92.50% for DR-DHS. Furthermore, the proposed LD method based on BP neural network has better transfer learning performance than that based on random forest or support vector machine.

- **Keywords:** Heating-network leakage diagnosis; BP neural network; Hydraulic working-condition simulation; Principal component analysis; Data feature transfer learning

Mahshab Sheraz, Juhea Kim, Juran Kim. *Nano/microplastics in indoor air: A critical review of synthesis routes for toxicity testing and preventative measure strategies*. Pages 274-304.

A future without plastic is difficult to imagine. Plastics are ubiquitous in every aspect of our lives, including cosmetics, clothing, packaging, toys, furniture, pigments, and carpets. Microplastic pollution of the oceans has had deadly consequences worldwide. However, few realize that micro-nanoplastics (MnPs) are also a significant contributor to airborne pollution. Indoor air pollution can be up to 100 times higher than outdoor air pollution. Every day, we inhale up to 130 small plastic particulates, and the concentration of MnPs in all environments is steadily rising. Several studies have investigated the

presence of MnPs in aquatic environments, but few have focused on indoor airborne MnPs. This study aims to investigate the origins, movement patterns, and repercussions of airborne MnPs. Additionally, it seeks to understand the mechanisms through which MnPs can infiltrate living organisms and impact their various body parts, potentially resulting in multiple diseases and significant health risks. Here, we discuss the synthesis of micro-nanoplastic routes of different polymers to prepare nanoplastics for examination of their toxicological effects by in vivo and in vitro testing. We also propose a unique remediation method to control MnP particles in indoor air using DTA (detect, trap, and adsorb) technology. We have outlined a variety of effective materials that can trap and adsorb nanoplastics. We recommend fabricating air filters using electrospinning devices and employing these efficient materials to create multifunctional filters for use in commercial air purifiers. We encourage researchers to open new paths in this research to control MnPs in indoor air. In future research, environmental suitability can be achieved through the adoption of biodegradable fibers and by considering the use of nanobiomaterials. Additionally, the potential release of MnPs and addressing the issue of material detachment from air filters in future research endeavors.

- **Keywords:** Micro-nanoplastics (MnPs); Indoor airborne plastic particles; Health impacts; Synthesis routes of MnPs; Remediation strategies (DTA technology)

Tao Hai, Amit Kumar, Saman Aminian, Basim Al-Qargholi, Naglaa F. Soliman, Walid El-Shafai. *Improved efficiency in an integrated geothermal power system including fresh water unit: Exergoeconomic analysis and dual-objective optimization*. Pages 305-323.

The single-flash geothermal cycle (SFGC) is not without its limitations, featuring drawbacks like diminished efficiency, restricted power generation capacity, and the incapability to yield multiple outputs concurrently. Furthermore, the SFGC requires a substantial water supply, potentially leading to adverse environmental consequences. In a concerted effort to enhance overall performance and facilitate the concurrent production of multiple valuable products, this study introduces a multigeneration system (MGS). By integrating additional subsystems into the SFGC framework, including a branched GAX cycle enabled by a thermoelectric generator (TEG), a domestic water heater (DWH), and a reverse osmosis unit, the objective is to surmount these limitations effectively. A thermodynamic and exergoeconomic analysis of the system is conducted and a bi-objective optimization is employed to minimize system cost and maximize exergy efficiency. The parametric study reveals that when degassing ranges are in the range of 0.2–0.37, the system product cost varies from $27.07/MWh to $28.44/MWh. In the optimized scenario there is a decrease of 67.7% in cooling provided by the system. This leads to an increase of 3.5% in generated electricity and a 3% increase in water purification compared to the base scenario. Through optimization the exergy efficiency of the system improves from 61.84% to 62.90% while the multigeneration gain output ratio (MGOR) decreases from 1.40 to 1.38.

- **Keywords:** Branched GAX/TEG cycle; Exergoeconomic; Multigeneration; NSGA-II; Pareto frontier

Moustafa M. Aboelmaaref, Jun Zhao, Mohamed E. Zayed, Yang Li, Lei Gu, Ahmed A. Askalany, Mohamed Ghazy, Ahmed S. Alsaman, Ehab S. Ali. *Design and dynamic numerical modeling of a hybrid reverse osmosis/adsorption-based distillation system driven by solar dish Stirling engine for enhanced performance and waste heat recovery*. Pages 324-338.

In light of green solutions to address the shortage of freshwater shortage, energy crisis, and climate change. Tri-generation renewable systems are recently efficient approaches

that can offer multiple energy outputs, such as heat, electricity, and distilled water. This paper presents a new hybrid freshwater production system driven by renewable energy for enhanced performance and waste heat recovery. This hybrid system proposes the utilization of reverse osmosis, an adsorption distillation system, and a solar dish Stirling engine (RO-ADS/SDSE). The cooperative concept is based on the re-desalination of the brine of the RO unit using an adsorption desalination system driven by the heat rejected from the SDSE, while the RO system is driven by the electrical energy produced by the Stirling engine. A mathematical model conducted in MATLAB coupled with EES package is developed to investigate the performance of the proposed RO-ADS/SDSE with and without pressure recovery (PR) mode at different salinity concentrations varying from 30000 to 50000 ppm at a constant feed pressure of 80 bar. The investigation is conducted based on the meteorological data of Tianjin, China. The results showed significant superiority in the performance of the proposed RO-ADS/SDSE system, as the annual freshwater production rate of the RO-ADS/SDSE with PR increased by up to 3000 m3 compared to 1700 m3 for the standalone RO system at a feed salinity of 45000 ppm and feed pressure of 80 bar. On a daily basis, the hourly permeating flow rate of the RO-ADS/SDSE with PR increased from 2.30 m3/h to 2.60 m3/h, and the permeate salinity decreased from 190 to 120 ppm. While the daily electricity consumption decreased from 5.20 to 4.40 kWh/m3. In conclusion, the proposed RO-ADS/SDSE system with PR can be considered a promising approach in maximizing the performance of desalination systems.

- **Keywords:** Solar desalination; Stirling engine; Solar dish; Adsorption desalination; Reverse osmosis; Cooling and freshwater dual production

Kun Wang, Baohua Cheng, Yuan Ren, Sen Wang, Ruilin Ji, Xiangy Kong. Flexible resource dynamic aggregation regulation method of virtual power plant to ensure more renewable energy generation. Pages 339-350.

The development of large-scale sustainable energy has affected the security of electricity systems. Virtual power plant (VPP) realize multi-energy synergistic complementation and efficient operation mainly with electricity. The paper proposed a flexible resource dynamic aggregation regulation method of VPP to ensure more renewable energy generation, which enables the efficient operation of multiple energy sources with electricity as the main source through collaborative and complementary measures. Firstly, the operating mode of VPP under market mechanisms is proposed, and the operating mechanism for VPP's participation in the market is established. Secondly, the types of flexible resources are identified, a cooperative game relationship between multiple autonomous agents within the power grid and VPP is formed to support an intelligent control method for VPP considering the complementarity of multiple energy sources and carbon emissions. Finally, a novel inverse cotangent compound differential evolution (NICCDE) algorithm is proposed by combining the innovative composite differential evolution algorithm with the tangent function, which realizes the flexible synergistic utilization of multiple energy sources. and reduces the training cost of the algorithm. Case studies from the conducted case study demonstrate the significant cost reduction achieved by the proposed method in comparison to conventional approaches when applied to VPP. Moreover, the utilization of this method enhances the precision and comprehensiveness of the search outcomes, thereby augmenting the overall effectiveness of the VPP system.

- **Keywords:** Dynamic aggregation; Flexible resources; New compound differential evolution; Virtual Power Plant

Gamze Soyturk, Onder Kizilkan, Mehmet Akif Ezan, C. Ozgur Colpan. *PVT integrated hydrogen production with small-scale transcritical power cycle*. Pages 351-360.

The objective of the present research is to examine the performance of an integrated hydrogen generation system based on solar power. The system is comprised of photovoltaic-thermal (PVT) panels, a transcritical Rankine cycle (tRC), and a hydrogen generation unit, namely proton exchange membrane electrolysis (PEME) process. Carbon dioxide (CO2), which is an environmentally friendly fluid, is used as the working fluid of tRC, where it is directly heated up in the PVT collector. To perform the performance assessment of the system, first, a dynamic simulation of the PVT is conducted based on data from August 17 of Izmir. After, energy and exergy analyses of the integrated system are carried out, followed by parametric analyses. According to the results, the maximum power obtained from the PVT is found to be 2.6 kW, the net energy generated from tRC is calculated as 0.8 kW, while the maximum H2 generation rate is 16 g/h.

- **Keywords:** PVT; CO2; Transcritical Rankine cycle; Hydrogen; PEM electrolyzer

Liang Wang, Sijia Ni, Hao Wang, Yiwei Sun, Shenguang Fu, Chenhao Tian, Yuechen Zhao, Jintuo Zhu, Rongkun Pan. *Influence of wettability alteration on water-blocking effect and gas desorption of coal*. Pages 361-374.

To resolve the water-blocking effect that reduces gas extraction after implementing hydraulic measures, alkyl polyglycoside (APG) and polyacrylamide (PAM) were used to treat coal samples to make wettability enhancement and medium wettability conversion, respectively. The contact angle, surface tension, solid surface energy, infrared spectroscopy, and high-pressure water injection desorption were performed to investigate the effects of reagents on the wettability alteration mechanism and desorption characteristics of coal. The results demonstrated that the surface energy, hydrogen bonds and oxygen-containing functional groups of coal alter wettability and gas desorption. The APG-treated coal samples exhibited increased surface energy, hydrogen bonds and oxygen-containing functional groups, whereas the PAM-treated coal samples demonstrated the opposite trend. The surface energy of coal reflects the state of APG and PAM molecules adsorbed on the coal surface, and the polar force of surface energy in coal follows a quadratic relationship with the volume of gas displacement desorption. Increasing the number of hydrogen bonds and oxygen-containing functional groups can improve wettability and decrease the interaction force between coal and methane molecules. This contributes to the lower atmospheric desorption of the APG-treated coal samples at high pressure. The total desorption volume of the APG-treated coal samples was 10–34% of that of the original coal at 0.737, 1.027, and 2.004 MPa gas pressures. The total desorption volume of PAM-treated samples at 2.004 MPa was 2.3474 cm3/g, which exceeded that of the original coal. Therefore, APG and PAM promoted gas desorption, and wettability enhancement yielded better results. This study provides an experimental approach for selecting the best reagent and excellent guidance for field applications.

- **Keywords:** Wettability enhancement; Medium wettability conversion; Water-blocking effect; Water injection; Gas desorption

Zhongheng Nie, Wei Gao, Haipeng Jiang, Fengyu Zhao, Guojie Zheng, Zongling Zhang. *Flameless venting characteristics of hydrogen explosion under the coupling of carbon dioxide and metal foam*. Pages 375-385.

To avoid the hazards of vented flame and external explosion caused by hydrogen-air explosion venting, the effects of metal foam and carbon dioxide on the characteristics of

vented flame, reduced overpressure, and external pressure are investigated. The results indicate that a combination of inerting (such as adding CO2) and venting technology is recommended to achieve the quenching of vented flames without increasing the reduced overpressure of hydrogen explosions. The effect of the thickness of metal foam and the concentration of CO2 on the length of vented flame is significant, but it only has a minor impact on the width. The laminar burning velocity of hydrogen decreases with the increase of the volume ratio of CO2, which weakened the chemical reaction and reduced overpressure and explosion severity (KG). The characteristics of the external explosion are revealed with the assistance of BOS images. When the venting diameter is 80 mm, the flameless venting efficiency is approximately at 53.33%. Finally, the criterion for heat transfer quenching of vented flames is discussed. The quenching mechanism during flameless venting of hydrogen explosions is analyzed, providing a basic reference for the safety design of hydrogen explosion protection.

- **Keywords:** Vented hydrogen-air explosion; Flameless venting; Vented flame; Heat transfer; Quenching mechanism

Haitao Lin, Junhong Liu, Ahmad A. Ifseisi, Mohammad Taghavi. *A novel bio-waste-driven multigeneration cycle integrated with a solar thermal field and atmospheric water harvesting cycle: An effort to mitigate the environmental impacts of the wastewater treatment plants*. Pages 386-403.

Poor management in the municipal waste disposal is a serious crisis for the health of the ecosystem and society. The implementation of the waste-to-energy projects can simultaneously recover the available energy in waste and significantly mitigate the environmental impacts of releasing waste into the environment. In this article, a novel bio-waste-driven multigeneration cycle (BW-MGC) integrated with a solar thermal field for the production of various valuable products from sewage sludge is introduced and evaluated (from thermodynamic, environmental and economic points of view). Herein, the biogas and syngas are obtained through the anaerobic digestion and gasification processes, respectively. Besides that, hydrogen energy and water production cycles are based on the water-gas shift reaction and atmospheric water harvesting cycle (AWHC) units, respectively. In the offered project, the heating capacity and a part of the electricity are obtained through the waste heat recovery system. The offered project provides a new process with a novel structure and configuration to produce useful products. Moreover, it can jointly address the simultaneous issues of energy, water, and environment. The offered plant can produce 18.1 MW of electricity, 18.72 l/h of water, and 0.9 kg/s of hydrogen fuel. The energy efficiency of the system in such design conditions was calculated as 36.12%, while the exergy efficiency was 40.9%. Further, the exergy sustainability factor, total products unit cost, and levelized total CO2 emissions are calculated as 0.5281, 0.05168 USD/kWh, and 0.2124 kg/kWh, respectively.

- **Keywords:** Bio-waste; Multigeneration cycle; Solar thermal field; Water-gas shift reaction; Atmospheric water harvesting; Wastewater treatment plants

Yiqi Liu, Jingyi Yuan, Baoping Cai, Hongtian Chen, Yan Li, Daoping Huang. *Multi-step and multi-task learning to predict quality-related variables in wastewater treatment processes*. Pages 404-416.

In wastewater treatment processes, lack of hardware sensors together with unacceptable dynamics, strong nonlinearity and large time delay often leads to a large number of key variables that are difficult to measure online accurately and timely, then frustrate safe operations of the processes. To accurately and timely capture the short-term behavior changes and trend development of critical variables, a novel neural network based soft-

sensing model is proposed to take full use of multi-task learning, direct multi-step prediction strategy and evolutionary algorithm to formulate a novel multi-task multi-step evolution (MTMSE) neural network. Firstly, single-output MTMSE (SO-MTMSE) neural network is used to realize the dynamic monitoring of a single variable. Moreover, by considering the spatiotemporal interaction among the data, the model is extended to multi-output MTMSE (MO-MTMSE) neural network to simultaneously realize multi-step prediction of multiple variables, thus providing a desired reference for optimizing the wastewater treatment processes. Finally, the proposed model is applied to the benchmark simulation model 2 (BSM2) and a full-scale wastewater treatment plant in Shenzhen. And the results show that the proposed dynamic soft sensor model outperforms the standard methods, such as autoregressive moving average model (ARMA) and multiple output gaussian process regression (MGPR).

- **Keywords:** Wastewater treatment; Multi-step prediction; Multi-task learning; Soft sensor; Neural network

Pu Huang, Jiali Fu, Dongya Qiu, Zhengjun Gu, Jian Sun, Yafei Guo, Chuanwen Zhao. *Experimental and kinetic study on the cyclic removal of low concentration CO2 by amine adsorbents in confined spaces*. Pages 417-427.

Amine-based adsorbents show great promise for removing low-concentration CO2 from environmental control and life support systems (ECLSSs) to ensure crew safety and task execution. In this work, granular silica gel (SG) support was prepared by the extrusion–spheronization (ES) method, and amine-based adsorbent pellets were synthesized by impregnating the SG support with tetraethylenepentamine (TEPA). Dynamic CO2 circulation removal tests were carried out under simulated confined space conditions in a 100 L chamber to evaluate the low concentration CO2 removal performance of the adsorbent pellets. The effect of operating parameters on CO2 removal performance was investigated by orthogonal experiments. CO2 adsorption capacity and removal efficiency were significantly affected by CO2 concentration and reaction temperature, while reaction rate was intimately depended on CO2 concentration and gas flow rate. The maximum CO2 adsorption capacity (0.55 mmol CO2/g), removal efficiency (83.25%) and reaction rate (0.93 mmol CO2/min) were achieved under the optimized conditions of 20 °C, 1.25%CO2 and 2 L/min. A kinetic equation well representing the correlation between reaction rate and CO2 concentration and gas flow rate was established. The TEPA-SG-ES adsorbent pellets exhibited satisfactory working stability, with CO2 removal efficiency and adsorption capacity slightly decreased from 83.25% and 0.55 mmol CO2/g to 75.45% and 0.53 mmol CO2/g in 10 cycles, respectively. The slight decay in CO2 adsorption performance was associated with the oxidative degradation of amine species in oxygenated atmosphere to form amide, nitrite and imine phases, and the change of amine distribution over the pellets in multiple cycles. Overall, the desired TEPA-SG-ES adsorbent pellets could be nice scavenger candidates for circulating purification of CO2 in confined spaces.

- **Keywords:** Amine-based adsorbent pellets; Low-concentration CO2 circulating removal; Confined spaces; Operating parameters; Orthogonal experiment

Yihuan Wang, Zhenwei Zhang, Siming Liu, Ailin Xia, Ruiling Li, Guojin Qin. *Importance sampling-based probabilistic performance modeling of low-, mid- and high-strength pipelines under coupling effect of hydrogen-induced damage and corrosion*. Pages 428-442.

In-service long-distance pipelines are a practical approach to implementing large-scale hydrogen transportation under the context of energy transition. However, the hydrogen-induced damage (HID) and corrosion would deteriorate the material properties and load-

bearing capacity of the pipelines. In the present study, the coupling effect of HID and corrosion are probabilistically incorporated into the mechanical characterization models for low-, mid- and high-strength pipelines. Spatiotemporal stochastic growth is modeled using the stochastic gamma processes with significantly affected defect geometric parameters to facilitate the uncertain performance status of pipelines. All unknown parameters of the proposed method can be inferred by inducing in-line inspection (ILI) data. The computational framework for importance sampling (IS) has been developed to estimate the system failure probability of corroded natural gas pipelines considering HID. Apply several programs to conduct probability analysis to demonstrate the applicability and effectiveness of the proposed method. The results demonstrate that HID affects the failure behavior and safety probability state of pipelines containing corrosion defects. The performances of various strength pipelines have significant differences in deterioration paths due to HID, causing additional maintenance or potentially disastrous consequences. The proposed method has been proven to capture the potential uncertainties of HID and corrosion on different-strength steel pipelines, which is beneficial for the lifecycle management of blended hydrogen natural gas pipelines.

- **Keywords:** Pipeline performance; Hydrogen-induced damage; Corrosion; Importance sampling; Probabilistic modeling

Ke Zhang, Jicui Cui, Yuxiao Zhou, AJY. Chen, Chuang Ouyang, Michael Palocz-Andresen, Ziyang Lou. *GHG emissions reduction patterns from waste sectors after forced source separation*. Pages 443-450.

Waste management is the bridge to balance resource conservation and climate change protection, and source separation is the pre-requirement to improve the recycling rate and normal human behavior. In this work, greenhouse gas (GHG) emission patterns were investigated from waste sectors from 2016 to 2021 in Shanghai, where force MSW source separation was first implemented in China since 2019. The GHG emission in the waste sector increased from 3.06 (2016) to 9.28 (2021) Mt CO2-eq due to the increase of waste disposal amounts from 7.35 (2016) to 11.83 Mt (2021). With the implementation of forced source separation in Shanghai on July 1st, 2019, the proportion of kitchen waste and water content decreased by 37.31% and 20.74% in dry waste, resulting in the increase of low heating value (LHV) by 99.39% (13,160 kJ/kg). The waste disposal system was optimized by employing resource recycling and anaerobic digestion of wet waste, and the corresponding GHG emission intensity decreased from 0.29 to 0.24 t CO2-eq per ton MSW. Three scenario analyses, including the Business-As-Usual (BAU) scenario, New Policy (NP) scenario, and Low-carbon (LC) scenario, were conducted to study the influence of the grid emission factor, wet waste disposal capacity, incineration power generation efficiency, and lower waste plastic proportion on the GHG emissions. The results showed that the GHG emission intensity would reach 0.28, 0.21, and 0.12 t CO2-eq per ton MSW in the BAU, NP, and LC scenarios. Optimizing waste disposal mode and reducing waste plastic from sourced separation was critical to reduce GHG emissions more effectively from the waste sector.

- **Keywords:** Waste management; GHG emission; GHG emission intensity; Forced source separation; Shanghai

Alex J. Frimpong, Gangfeng Tan, Yuxiao Zhang, Jiedong Ye, Philip K. Agyeman, Sampson K. Kyei, Isaac O. Olayode. *Experimental investigation supported by artificial neural networks (ANNs) for predicting the heating performance of a cyclone separator coupled with induction heating coil*. Pages 451-474.

This paper proposes a novel dust separation and thermal inactivation system that couples an electromagnetic induction heating coil with a cyclone separator. The idea is aimed at

the thermal inactivation of potential microorganisms (viruses and other pathogens) associated with dust-laden gas streams, particularly from road surfaces. The integrated system was tested in an experimental setup as a proof-of-concept investigation at different cyclone-induction heating temperatures of 100–400 °C (373–673 K) and air discharge flow velocities of 5–30 m/s. In addition, the influence of operating parameters such as cyclone heating temperature (as induction heating inputs), inlet air velocity, and heating time on the efficacy of the induction heating process were investigated. The time-averaged temperature measurements along the axial direction (z-down) showed predominant temperature fluctuations in the cylinder and cone sections for all cases, especially when the gas plummets down the cyclone. Temperature was highest in the conical section (z = 525 mm) at 320 °C (593 K) at 5 m/s and lowest in the outlet section (z = 375 mm) at 185 °C, which was expected. The results show that inlet air velocity plays a crucial role in affecting temperature dynamics. Conclusive results indicate that with increasing temperature, pressure drop decreases significantly. Along with the experimental results, multiple regression indices using an Artificial Neural Network (ANN) modeling were used to predict the cyclone's induction heating performance, showing good prediction quality in terms of the mean square errors (MSE and RMSE) and the correlation coefficient R2: 0.99. The study demonstrates the technical viability of integrating induction heating coil to a cyclone separator for wide temperature applications.

- **Keywords:** Cyclone separator; Electromagnetic induction heating; Thermal inactivation; Artificial neural networks; Heating performance

Shadrack K. Musyoka, Ahmed S.G. Khalil, Shinichi A. Ookawara, Ahmed E. Elwardany. *Investigating C3 and C4 esters and alcohols in a diesel engine: Combined influence of carbon chain length, oxyfuel type, and oxygen content*. Pages 475-486.

Diesel engines fueled by liquid fuels will continue to dominate the transportation and heavy machinery application market despite the advancement of other technologies. Studies have yet to be conducted to investigate the combined influence of carbon chain length, oxyfuel type, oxygen content, and blending ratio of esters and alcohols as additives in diesel fuel. The present study addresses this by preparing two sets of experiments using three-carbon (C3) and four-carbon (C4) additives, one at an equal blending ratio of 4% and the other at an equal oxygen mass content of 1.94%. Although the additives caused up to 24.84% rise in brake specific fuel consumption at low load, the value diminished to 7.86% at medium load and 11.63% at high load. The C4 fuels were found to have better NOx reduction potential than the C3 fuels. However, most additives significantly increased CO emissions, except for EE4.9 (4.9% ethyl ethanoate and 95.1% diesel), leading to 3.7% and 7.1% lower CO emissions than neat diesel at low and medium loads, respectively. Smoke emissions were also reduced by up to 32.84% when oxygenated additives were used. Although all blends tested are promising fuel alternatives in a diesel engine, EE4.9 provided the most suitable trade-off between engine performance and emissions.

- **Keywords:** Esters; Alcohols; Emissions; Carbon chain length; Diesel engine

Joël Placide Kouer, Pierre Meukam. *Power generation scenarios for Cameroon: Valorisation of biomass for the reduction of electricity transmission and the mitigation of greenhouse gas emissions by 2050*. Pages 487-510.

This work aimed at solving the environmental problem of the hottest greenhouse gas reduction. The paper identifies the energy electricity demand, proposes solutions, and calculates the greenhouse gases emitted in each of the interconnected networks available

in Cameroon. For a total production estimated at 1292 MW, the country's electricity production depends heavily on hydropower plants (57%), thermal power plants (42%), and only 1% of biomass. Specifically, biomass would contribute to 40% of the supply of the demand if it is sufficiently exploited. Hydroelectricity needs transmission for long distances. The electricity demand in the median economic scenario is the basis of this study. GHGs were calculated using the tool MESSAGE. The results of this study show that it will be possible, without taking into account the fact that biomass is clean energy, to avoid 462 kt of CO2eq and 14 kt of CO2eq for South Interconnected Network and East Interconnected Network respectively. The amounts of CH4, SO2, and NOx are not statistically significant. This study takes into account the main existing energy sources in the country. The specificity of this study is to treat the three interconnected networks of the country separately. The use of biomass in local power plants was proposed to reduce dependence on fossil fuels. This study shows that to reduce the GHG emission and the loss of electricity due to its transmission in the country, it is better to use biomass instead of fossil fuels for the production of electricity in Cameroon.

- **Keywords:** Power Generation technology; Biomass; Greenhouse gas emissions; Electricity production in Cameroon

Mohamad Abou Houran, Sayed Fayaz Ahmad, Tirumala Uday Kumar Nutakki, Manoj Kumar Agrawal, Ayman A. Ghfar, Jong Boon Ooi, Aliashim Albani, Shaobo Xie. *Numerical simulation and 4E analysis of a steam methane reforming-based multi heat recovery process, producing electricity, methanol, fresh water, heating, and coolant*. Pages 511-534.

Natural gas power plants play a pivotal role in power generation; nevertheless, their waste heat contributes to diminished thermodynamic efficiencies and the release of carbon dioxide emissions. One primary approach involves implementing effective heat recovery strategies to generate various products. The present study suggests a novel approach to heat recovery in different stages utilizing series and parallel arrangements within an environmentally friendly design to enhance controllability while expanding the range of products. The present study includes a steam methane reforming process, a Kalina cycle, a multi-effect desalination unit, a methanol synthesis unit, two organic Rankine cycles, and two ammonia Rankine cycles. The primary objective of this system is to efficiently and concurrently produce electricity, hot water, chilled water, fresh water, and methanol. The findings reveal that the newly devised process exhibits energy and exergy efficiencies of 47.55% and 50.58%, respectively, while the total unit cost of products amounts to 7.69 $/GJ. From an environmental perspective, the results indicate that the proposed structure exhibits a total net emission of 87.1 × 103 kg/h and a CO2 footprint of 0.22 kgCO2/kWh. Ultimately, the economic assessment elucidates that the fixed investment cost, total investment cost, total annual cost, and net present value are equivalent to 373.0 M$, 496.1 M$, 207.5 M$, and 598.6 M$, respectively.

- **Keywords:** Energy analysis; Exergy analysis; Poly-generation; Thermal integration; Methanol; Fresh water; CO2 footprint

Taynara O. Silva, Jesus Fernandez-Cascán, Julia Isidro, Cristina Saez, Marcos R. V. Lanza, Manuel A. Rodrigo. *Degradation of real lindane wastes using advanced oxidation technologies based on electrogenerated hydrogen peroxide*. Pages 535-543.

In this work, hydrogen peroxide (H2O2) is produced using an optimized electrochemical cell equipped with a gas diffusion electrode (GDE) as cathode, reaching efficiencies as high as 20.1%, when operating in a single compartment configuration, which increases up to the range 50–60, when a proton exchange membrane is used to separate the anodic and cathodic compartments, pointing out the great significance of the anodic

oxidation of H2O2 and the scavenging effects of the oxidants produced on the anode surface. As compared to previous materials tested, the GDE implemented in this cell underwent a more sustainable manufacturing procedure and exhibited an outstanding performance. The H2O2 produced electrochemically is dosed to the real leachate of an industrial dump, strongly polluted with derivatives of lindane. This waste is associated to the operation of a large facility in the seventies and contains different isomers of hexachlorocyclohexane and other chlorinated hydrocarbons, produced during the ageing of the dump. Effects of the addition of iron (II) sulfate salts and irradiation of UVC were also evaluated. All electrochemically-assisted technologies evaluated (named as chemical (EACO), Fenton (EAFO), photolysis (EAPO) and photo-Fenton (EAPFO) oxidations) were able to successfully remove the pollutants, although with important differences in the efficiencies reached. Results demonstrate that EACO, that is, oxidation by molecular H2O2 is the most effective treatment for the treatment of this type of wastes, pointing out that activation of H2O2 to hydroxyl radicals, either by electrochemically assisted Fenton or photolysis is not positive for this waste. As well, among the different pollutants contained in the raw waste, removal of hexachlorocyclohexane (HCHs) and non-chlorinated volatile organic compounds (VOCs) stands out (both groups being the primary species contained in the wastes). These results are very important not only because of the outstanding productions of H2O2 reached with the novel approach of electrochemical cell used, but also because of the implications of the mechanistic understanding of the attack of H2O2 species in the design of a full-scale application to remediate this real important problem.

- **Keywords:** Hydrogen peroxide; Hexachlorocyclohexanes; Electro-Fenton; Electrolysis; Radicals

Wenlong Zhang, Qian Xie, Jia Jia, Gonghua Jiang, Changhai Li, Yanming Ding. *Effect of accelerated weathering on pyrolysis kinetics and ignition characteristics of typical thermal insulation materials*. Pages 544-553.

Thermal insulation materials are widely installed on external walls because of their excellent properties. However, thermal insulation materials are often exposed to air and sunlight as external facades fall off, which can lead to weathering and potential fire risk. Especially, weathering may cause changes in pyrolysis and combustion characteristics of thermal insulation materials, which is of great significance for understanding fire. To simulate real exposure conditions, typical thermal insulation materials (expanded polystyrene) were weathered by accelerated weathering for 25, 45, 90, 135 and 180 days. Pyrolysis characteristics of unweathered and weathered materials were researched by thermogravimetric analysis, Fourier transform infrared (FTIR) spectrometric technique and cone calorimeter experiments. The kinetic parameters were estimated and optimized using Coats-Redfern and Shuffled Complex Evolution methods. Subsequently, the correlation between weathering time and kinetic parameters was obtained. The functional groups were detected by FTIR. Finally, the ignition time was measured. The results showed that the color of materials changed and the chalking appeared as accelerated weathering increased. Activation energy decreased from 324.44 kJ/mol to 91.04 kJ/mol, and pre-exponential factors reduced from 52.31 lns−1 to 10.72 lns−1. The intensity of vibration bands was strengthened. Ignition time was shortened by 119 s, indicating that weathered EPS is more easily ignited.

- **Keywords:** Thermal insulation materials; Fire; Pyrolysis; Accelerated weathering; Kinetic parameters; Ignition time

Ce Wang, Yuling Lü, Tianxu Ye, Li Chen, Limin He. *Investigation on the mechanism of air/condensate bubble flotation of emulsified oil droplet*. Pages 554-565.

Crude oil droplets in oilfield-produced water are highly emulsified, and the poor attachment between gas bubbles and oil droplets limits the effectiveness of oil-water separation during flotation processes. This paper proposes a new surface-functionalized bubble called a condensate bubble and evaluates its flotation performance based on surface properties and adhesion theory mechanism to address this issue. The surface chemical properties of the oil droplets were characterized using X-ray photoelectron spectroscopy (XPS), contact angle measurement, and zeta potential. Induction time and flotation tests were conducted to compare the attachment effects between air or condensate bubbles and emulsified oil droplets. The interaction forces were calculated using DLVO and extended DLVO theory. The experimental results showed that crude oil contains functional compounds containing oxygen that make it tough to float. However, the contact angle between the oil surface and condensate bubble was greater than 150°, demonstrating that the condensate liquid bubbles have better hydrophobicity than air bubbles. The micro-flotation experiments indicated that condensate bubbles have a strong collection capacity for emulsified oil droplets, which was confirmed by induction time tests. In 70 mM NaCl brine, the oil removal efficiency of condensate bubble flotation could reach 82%, which was a 30% improvement compared to air bubble flotation. However, DLVO theory failed to predict the flotation with a concentration higher than 10 mM NaCl. The extended DLVO theory accounted for hydrophobic interactions, which were observed due to similar solvent extraction and hydrophobicity of the condensate liquid film. As a result, the condensate bubble-oil droplet system exhibited stronger hydrophobic attraction, successfully confirming and illustrating the superiority of the condensate bubble in flotation.

- **Keywords:** Oil-water separation; Condensate bubble flotation; Homologous extraction; Induction time; Extended DLVO theory

Seyed Sajad Hashemi, Mehdi Abbasi-Riyakhuni, Joeri F.M. Denayer, Meisam Tabatabaei, Mortaza Aghbashlo, Keikhosro Karimi. *Efficient bioremediation of distillery and dairy wastewaters: A three-stage biorefinery for high-quality aquaculture feed and bioenergy generation*. Pages 566-574.

The present study is motivated by the need to address the environmental issues related to dairy and ethanol plant wastewaters and to generate valuable products, including mycoprotein and bioenergy, through a novel three-phase fungi-based biorefinery. In the initial phase of the biorefining process, the cultivation conditions of Aspergillus oryzae were optimized. The objective was to maximize mycoprotein production using wastewater as a resource. The effluent generated during the first phase of the biorefinery underwent the second phase, where it was subjected to cultivation with Neurospora intermedia. In the third phase, the effluent obtained from the fungal growth underwent anaerobic digestion as a final treatment step, producing 306 NmL methane/g VS. This three-phase biorefinery contributed to a remarkable reduction in the chemical oxygen demand level of the wastewater by 56.8%, 11.6%, and 28.1% in each respective phase. Overall, the three-phase biorefinery process yielded promising results, generating 17.8 kg of mycoprotein and 5.0 Nm3 of biomethane per cubic meter of wastewater. The mycoprotein obtained through this process contains noteworthy quantities of essential amino acids, fatty acids, and minerals. These characteristics open up opportunities for substituting conventional feed in aquaculture with the produced mycoprotein.

- **Keywords:** Fungi-based biorefinery; Fish feed; Biogas; Mycoprotein; Environmentally friendly valorization

E. David. *Composites derived from co-pyrolysis of residual biomass with aluminium slag as effective materials for volatile organic compounds removal.* Pages 575-587.

Co-pyrolysis is an important method to transform hazardous waste into new materials, and composites based on biochar and metal oxides could constitute new types of adsorbents for volatile organic compounds (VOCs). In this study, residual biomass (corn cob, rapeseed and walnut shell) was co-pyrolyzed at 650OC with aluminum slag (AlS), and different composites were synthesized. Biocomposites have been used as adsorbents for the removal of VOCs (such as acetone and toluene). The results showed that the biocomposite obtained from corn cob and AlS has a higher adsorption capacity for acetone, while the composite obtained from walnut shell and AlS showed a higher adsorption capacity for toluene. All prepared composites showed a higher adsorption rate than the corresponding pure biochars. After eighth cycles of adsorption/desorption, the results obtained showed the sample AlS650-Na/BCCC presented a good adsorption performance for acetone (318 mg/ g) in the first three cycles, and then the adsorption capacity decreased slowly, with the increase in the number of adsorption cycles. However,the adsorption capacity of 254.41 mg/g was still high after the eighth cycles.A similar behavior was presented by the AlS325-Na/BCWS composite for toluene adsorption.Therefore,AlS/BC composites could be used as a potential adsorbents in VOCs removal.

- **Keywords:** Co-pyrolysis; Aluminium slag; Biochar; Composite; VOCs removal

Yunfei Huang, Guojin Qin, Ming Yang. A risk-based approach to inspection planning for pipelines consider*ing the coupling effect of corrosion and dents*. Pages 588-600.

RBI, referring to a risk-based approach to inspection planning, is an established pipeline integrity management method. Both corrosion and dents are the primary threats to pipeline integrity. However, they are often treated separately in RBI without considering their interactions. This coupling may lead to a synergic effect on integrity degradation. The present study proposes an RBI planning framework for pipelines considering external corrosion and dents. Time-dependent pipeline deterioration by dents and corrosion is modeled probabilistically using a Dynamic Bayesian Network (DBN), in-line inspection (ILI) data, and corrosion propagation knowledge. Two failure scenarios (leakage and burst) are considered. The hybrid method, integrating Monte Carlo Simulation (MCS) and Latin Hypercube Sampling (LHS) technique, estimates the pipeline's Probability of Failure (PoF) over time. The pipeline failure risk is quantified by monetizing the Consequence of Failure (CoF). An optimization model of loss-maintenance total expected cost is introduced to determine the optimum inspection period using maximum acceptable risk (MAR) and the lowest total expected cost. A cost-benefit analysis (CBA) is finally implemented to choose appropriate risk reduction measures. The proposed framework is robust and well-validated by a case study on an in-service pipeline.

- **Keywords:** Pipelines; Corrosion; Dents; Risk-based inspection; Dynamic Bayesian network

Juqiang Feng, Feng Cai, Huachen Li, Kaifeng Huang, Hao Yin. *A data-driven prediction model for the remaining useful life prediction of lithium-ion batteries*. Pages 601-615.

Accurate prediction of remaining useful life (RUL) can ensure the safety and reliability of power batteries during operation, reduce the failure rate and operating costs, and enhance user experience. However, battery degradation is a complex, nonlinear dynamic process that is difficult to fully comprehend and predicting RUL remains a significant

challenge. To address this issue, the hybrid data-driven prediction model PCA-CNN-BiLSTM was proposed in this paper, which combines principal component analysis (PCA), convolutional neural network (CNN), and bi-directional long short-term memory (Bi-LSTM) network. PCA was applied to downscale and whiten the health factor (HF) to maximize the extraction of important features of lifespan decay, while reducing the correlation between features. The convolution kernel of the CNN was used to explore the local region feature information of the input information and search for the common patterns among the neighboring data. Additionally, the model parameters and computational efforts were reduced through pooling. Finally, battery RUL prediction was achieved using Bi-LSTM, which has the advantages of effectively enhancing model accuracy and reducing the risk of over-fitting by taking into account both past and future data. The performance of the proposed model was evaluated utilizing NASA and CALCE's battery datasets, and the results suggest that it exhibits a high level of accuracy across various datasets. Compared to other methods, the PCA-CNN-BiLSTM method has the best performance indicators for predicting battery RUL, including RMSE, MAE, MAPE, RULe and DOL. This indicates that the proposed model has better fitting performance, accuracy, robustness, and generalization ability.

- **Keywords:** Lithium-ion batteries; Remaining useful life; Health factor; Principal component analysis; Convolutional neural network; Bi-directional long short-term memory

Yabing Song, Sayed Fayaz Ahmad, Mohamad Abou Houran, Manoj Kumar Agrawal, Tirumala Uday Kumar Nutakki, Masoom Raza Siddiqui, Aliashim Albani, Qiaolin Su. *Multi-variable study of a novel multigeneration system using biogas separation unit and LNG cold energy utilization, producing electricity, cooling, heat, fresh water, liquid CO2, biomethane, and methanol*. Pages 616-638.

Biogas fuel has gained recognition as a highly suitable alternative to fossil fuels, attributed to its renewable nature and remarkable energy density. Biogas fuel utilization facilitates the integration of combined energy systems equipped with multi-generational structures, rendering them suitable for long-term planning and management. Hence, this study presents a unique approach to using biogas for multigeneration, exhibiting enhanced thermodynamic efficiencies and negative carbon dioxide emissions. To achieve the stated objective, an innovative system is devised that involves the utilization of a biogas separation unit in integration with several other components, including a LNG cold energy utilization unit, an ammonia Rankine cycle, a desalination unit, a Kalina cycle, a solid oxide electrolyzer cell, a biomethane combined cycle, and a methanol synthesis unit. The newly devised configuration is simulated through the Aspen HYSYS software and assessed from energy, exergy, environmental, and economic considerations. Based on the research findings, the suggested methodology exhibits energy and exergy efficiencies of 91% and 83%, correspondingly. Furthermore, the evaluation of the entire unit cost of the product and the levelized energy cost reveals values of 4.81 $/GJ and 0.033 $/kWh, respectively. The carbon dioxide emission intensity of the newly implemented process is calculated to be − 0.1041 kg/kWh. The economic aspects reveal a favorable net present value of 1470.6 M$ and a payback period of 5.29 years.

- **Keywords:** Polygeneration; Biogas separation; LNG cold energy; Methanol synthesis; Liquid CO2; Negative CO2 emission

Guo Qing, Ren Wanxing, Meng Xianliang, Xia Hongchun, Shi Jingtai. *An investigation into the morphological distribution of the temperature field in loose media and its underlying principles of evolution*. Pages 639-647.

The spontaneous combustion of coal in goaf has important implications for the safe mining of working faces; hence, it is crucial to prevent and control such occurrences. Here, we establish an experimental system to investigate the morphological distribution, evolution, and migration process of the temperature field of the thermal core area in systems with various particle sizes. Furthermore, we propose a high-temperature-region inversion method based on the morphological evolution model of the temperature field. Our experimental results demonstrate that particle size is a critical factor influencing the temperature field morphology under a given heating condition. During the heating stage, the isothermal surface within the thermal core area forms an ellipsoidal shape, with a transverse section comprising concentric circles, and a longitudinal section comprising ellipses. During the heat dissipation stage, the isothermal surface of the small-particle-size system encircles the thermal core area from the upper direction downwards, while the isothermal surface of the large-particle-size system encircles the thermal core area from the lower direction upwards. Moreover, the thermal core area of the large-particle-size system migrates upwards, while the thermal core area of the small-particle-size system migrates a shorter distance. Finally, we used a geometrically simplified temperature field in loose media to propose a high-temperature-region inversion method, which was verified by experiments. This study is crucial for understanding the distribution and evolution of temperature fields in loose media and predicting the formation and development of high-temperature regions.

- **Keywords:** Coal spontaneous combustion; Loose media; Temperature field; Morphological evolution; Temperature field inversion

Rui Shang, Peiyu Shi, Yong Yue, Farshid Sardari. *Simulation and multi-aspect investigation of a geothermal-based power, hydrogen, oxygen, and fresh water production integrated into a flue gas-driven combined power plant*. Pages 648-668.

This paper introduces and evaluates a novel multi-generation structure that employs geothermal energy and utilizes waste heat from flue gas. This innovative structure includes a combined flash and binary geothermal system, a multi-effect desalination subsystem, a proton electrolyte membrane electrolyzer, a steam Rankine cycle, and a dual-pressure organic Rankine cycle. The proposed plant is evaluated from energy, exergy, economic, and environmental viewpoints. Moreover, a detailed parametric analysis is performed to study the effect of different parameters on the system performance. Results obtained demonstrate that this proposed process can generate 21.93 kg/s of fresh water, 346.1 kg/h of green hydrogen, 2739 kg/h of green oxygen, and 19,090 kW of power. Furthermore, the overall energy, exergy, electrical efficiencies, and total unit cost of the product for this new process are determined to be 16.44%, 53%, 8.7%, and 4.56 $/GJ, respectively. Additionally, through exergy analysis, it is established that the Proton Electrolyte Membrane Electrolyzer boasts the highest efficiency within the proposed process, with an exergy efficiency of 88.84%. Its contribution to the total irreversibility of the system is calculated at 1%. Moreover, the analysis reveals that the combined flash and binary geothermal system is the most significant contributor to irreversibility, accounting for 58% of the total, while turbine 2 represents 35.53% of the system's overall irreversibility. From an environmental perspective, employing this proposed process for power generation leads to an annual saving of 44,482,754 liters of petroleum. From an economic standpoint, the total investment cost of the proposed process amounts to $20,743,728. Among the subsystems, the combined flash-binary geothermal system incurs the highest investment

cost, representing 41% of the total, while the proton electrolyte membrane electrolyzer has the lowest cost share at 6%.

- **Keywords:** Geothermal energy; Flue gas waste energy; Aspen HYSYS simulation; Multigeneration process; Fresh water; Hydrogen

Mohamed R. Elmenshawy, S.M. Shalaby, Ahmed I. Elshinnawy, Tamer A. Gado. Groundwater desalination for agricultural purposes using reverse osmosis and nanofiltration technologies: Case study wadi El-natrun, Egypt. Pages 669-685.

The current study aims to assess the water quality in Wadi El-Natrun (Egypt) for agricultural purposes and to design an optimal desalination system that considers the water quality, the power consumption, and the total cost of the system. Water quality was evaluated based on four indices: electrical conductivity (EC), sodium adsorption ratio (SAR), residual sodium carbonate (RSC), and toxicity risk of three ions (sodium, boron, and chloride). The proposed desalination systems are single- and double-stage hybrid systems based on reverse osmosis (RO) and nanofiltration (NF) membranes. The performance of these systems was evaluated and compared in terms of the quality of permeated water for agricultural uses. The net present value (NPV) was also used as an economic criterion to determine the optimal system for agricultural purposes from an economic point of view. The results showed that most of the wells investigated are not suitable for direct irrigation before treatment due to problems of salinity, sodium adsorption, and chloride toxicity. Reverse osmosis membranes have proven to be superior to nanofiltration for producing high-quality water for agricultural purposes. However, single-stage systems with nanofiltration membranes are the most cost-effective option for most of the wells investigated in the study; they are the best for 30 out of 47 wells. It is also concluded that the use of nanofiltration desalination technology for irrigation purposes is a feasible solution that would encourage investors to expand reclamation projects in the Western desert in Egypt.

- **Keywords:** Desalination; Reverse Osmosis; Nanofiltration; Water quality assessment

Norafneeza Norazahar, Tamarai Malar Ambikabathy, Rafiziana Md Kasmani, Arshad Ahmad, Aishah Abd Jalil, Tuan Amran Tuan Abdullah, Mohd Fadhzir Ahmad Kamaroddin. *Hydrogen application and its safety: An overview of public perceptions and acceptance in Malaysia*. Pages 686-698.

This paper presents a survey assessing factors contributing to the public acceptance of hydrogen as a fuel for vehicles in Malaysia. For the survey, a set of questionnaires was prepared in Google Forms and distributed to respondents through social media (WhatsApp, Facebook, Messenger, and Telegram). The survey was conducted during the movement order control in Malaysia due to the global pandemic, and the responses were collected from November to December 2021. One hundred seventy-six local respondents voluntarily participated in the survey. The responses were analysed using non-parametric statistical tests in the Statistical Package for the Social Sciences (SPSS). The highest number of respondents from the 18–25 age group is 101 (57.39 per cent), followed by 26–35 (26.7 per cent) and 36–45 (7.95 per cent). The statistical analysis of the survey shows that socio-demographics is a factor influencing public acceptance. The Spearman correlation test shows a positive correlation between Malaysia's environmental awareness and the potential to use a hydrogen-powered car; hence, there is a good chance of Malaysian acceptance of using hydrogen as fuel. Safety and public perception of hydrogen-powered cars also indicate a positive correlation, where the R-values for all questions are more than 0.5, indicating that safety is a factor that shapes public

acceptance. Although the number of samples does not represent the population, it provides a reasonable basis to examine the influencing factors of public acceptance of hydrogen as a fuel for vehicles.

- **Keywords:** Correlation study; Hydrogen fuel cell; Hydrogen safety; Public acceptance; Transportation

Lianzhuo Zhang, Xiaobing Zhan, Xingqing Yan, Xiaoyang Liu, He Liang, Jianliang Yu. *The differences in quenching characteristics of H2/Air deflagration and detonation propagation in the T-shape pipeline*. Pages 699-711.

Bifurcated pipeline is a typical structure in industrial and transportation; paying attention to the propagation of explosions in it and taking measures to prevent explosions are extra important. The deflagration and detonation propagation characteristics of stoichiometric H2/Air mixture were investigated under initial pressure ranging from 25 kPa to 45 kPa based on the T-shape pipeline experimental system; the effects of flame arrester locations and structure were further experimentally explored under different initial pressures. Differences in the velocity characteristics of deflagration and detonation in the T-shape pipeline and the quenching characteristics after passing through differently positioned flame arresters were found. The results show that enhanced turbulence caused by the change in cross-section at the T-junction promotes the deflagration propagation, and the diffraction generated by the corners at the T-junction suppresses the detonation. Moreover, the velocity changing magnitude (A) indicated that deflagration accelerates faster and detonation attenuation reduces as initial pressure rises in the branch. The experimental results of the flame arrester installed in the pipeline suggested that deflagration and detonation slow down, and installing locations influence quenching pressures and decelerating reduction magnitude (S). According to the pressure signals, there are four flame stages: none, weak, rises sharply to peak, and fluctuations decline. The quenching pressure of detonation is higher than deflagration when the flame arrester is in the same position. Deflagration has higher quenching pressure of 60 kPa and S of 84.5% when the flame arrester is installed in the branch; Detonation has higher quenching pressure of 80 kPa when the flame arrester is installed in the straight while a higher S of 83.3% in the upstream. The cavity experiments of the flame arrester confirmed that deflagration deceleration comes from the combined effects of turbulent acceleration due to cross-section changes and deceleration due to heat exchange in the flame arrester; Detonation deceleration is due to the obstruction of the expansion wave caused by the gradual-expansion entrance of the flame arrester.

- **Keywords:** Bifurcated pipeline; Quenching characteristics; Propagation characteristics; Deflagration; Detonation; Crimped-ribbon flame arrester

Yiquan Liu, Dhanendra Kumar, Zhitao Chen, En-Hua Yang. *Qualitative and quantitative characterization of metallic aluminum in municipal solid waste incineration bottom ash*. Pages 712-724.

The reaction of alkaline solution and metallic aluminum present in municipal solid waste (MSW) incineration bottom ash (IBA) generates hydrogen gas. Thus, it is crucial to characterize the metallic aluminum in IBA for its safe utilization and proper disposal. However, the inherent inhomogeneity of IBA, random distribution of metallic aluminum in IBA grains, presence of aluminum in compound forms, and lack of reliable quantitative characterization techniques pose significant challenges to the holistic understanding of metallic aluminum in IBA. This research aims to address these questions systematically and present a comprehensive understanding of metallic aluminum in IBA. A classification strategy based on mineralogical and particle size basis is adopted to minimize the inhomogeneity of IBA. Furthermore, the spatial distribution of metallic aluminum in IBA is

studied through SEM/EDS of the IBA grains cross-sections of different particle sizes and mineralogical classes. Subsequently, a modified in-house designed collecting gas over liquid setup was developed for an easy and reliable quantitative characterization. The metallic aluminum content was the highest for 0.3–1.18 mm and lowest for < 0.3 mm range, and within a given mineralogical class, the metallic aluminum content decreases with decrease in particle sizes. The microanalysis of cross-sections of IBA grains showed that the aluminum is present as aluminum alloy formed during incineration or in oxide form, majorly in fine fractions (< 0.3 mm). The current study seeks to provide a complete picture of metallic aluminum distribution in IBA.

- **Keywords:** Municipal solid waste; Incineration bottom ash; Classification; Characterization techniques; Metallic aluminum; Hydrogen gas

Qiuye Jin, Qiong Duan, Dingyu Ji, Jie Chang, Zhaomin Tang. *Reaction mechanism, degradation pathway and toxicity assessment of NH4+ enhanced potassium ferrate removal of levofloxacin*. Pages 725-734.

Considering that ammonium ion (NH4+) was widely distributed in natural water and many sewage, it was of great practical significance to study NH4+ enhanced potassium ferrate (Fe(VI)) to rapid removal of levofloxacin (LEV) from water. In this experiment, firstly, the reaction kinetic of NH4+ enhanced Fe(VI) removal of LEV was studied, and the results showed that the enhanced removal reaction conformed to the second-order kinetic equation. When pH ≤ 9, the second-order rate constant kapp was linearly related to NH4+ dosage, but when pH= 10, the above linear relationship was broken, and the slope of the fitting line would change toward a smaller trend. Subsequently, tert-butanol (TBA) and Methyl phenyl sulfoxide (PMSO) were used as probes for·OH and high-valent iron-based intermediate (Fe(V)/Fe(IV)) respectively, which further revealed the reaction mechanism that NH4+ enhanced Fe(VI) to remove LEV as follows: NH4+ could promote Fe(VI) to produce a large amount of Fe(V)/Fe(IV), thus accelerating the degradation of LEV. In addition, 10 degradation intermediates of LEV were identified by quadrupole time-of-flight tandem ultra-performance liquid chromatography mass spectrometer (Q-TOF LC-MS), and then combined with density functional theory (DFT) calculation, two possible degradation pathways were inferred. Through the luminescence inhibition experiment of Vibrio fischeri and the toxicity evaluation of ECOSAR, it could be concluded that in the process of NH4+ enhancing Fe(VI) to remove LEV, the toxicity of the solution showed a trend of increasing first and then decreasing, and its toxicity was effectively improved and reduced after full oxidation. Finally, the experiments in actual water showed that it was feasible to use NH4+ in actual water to enhance Fe(VI) for rapid removal of LEV.

- **Keywords:** Potassium ferrate; NH4+ enhancement; Removal mechanism; Degradation pathway; Toxicity assessment

Zheng Li, Qiping Zheng, Kaicong Cai, Lin Yang, Jinkun Yang, Hongwei Sun, Changqing Liu, Weifang Zhang, Yuyi Zheng, Chunshan Wu. *Degradation of ribavirin by potassium ferrate(VI): Kinetics, degradation pathway and toxicity assessment*. Pages 735-743.

The degradation of ribavirin(RBV) by ferrate(Fe(Ⅵ)) was systematically investigated for the first time by experiment and degradation process fitting. The results indicated that the reaction between Fe(Ⅵ) and RBV is pH dependent and followed second order kinetics. The species-specific rate constants of the Fe(Ⅵ) species(HFeO4-) were higher than FeO42- species when react with RBV. Fe(VI) made significant contribution to the removal of RBV. Liquid chromatography-triple quadrupole mass spectrometry(LC-TQ-MS) was used to determine the intermediate of RBV which degradated by Fe(Ⅵ), in order to infer its main degradation pathway. This study used Dual Descriptor and Fukui function to

calculate the active sites of RBV and its intermediates during the degradation of RBV by Fe(Ⅵ), then verified their accuracy with actual reaction sites deduced based on LC-TQ-MS data. The results showed that Dual Descriptor prediction was more accurate than Fukui function in the process of RBV degradation by Fe(Ⅵ). Some common anions in natural waters, such as SO42-, NO3-, Cl- and CO32- had no effect on the removal of RBV by Fe(Ⅵ). 50 mg/L HA reduced the 120 min removal efficiency of RBV by 15.07%. Both toxicity analysis by ECOSAR software and E. coli toxicity experiments showed that Fe(VI) achieves toxicity reduction of RBV. This study indicated that Fe(Ⅵ) can effectively remove RBV from water and using Dual Descriptor to analyze the active sites of intermediates in the RBV degradation pathway can enhance the rationality of predicting the reaction pathway.

- **Keywords:** Ferrate(Fe(Ⅵ)); Ribavirin; Reaction products; Dual Descriptor

Boris V. Ivanov, Ruslan M. Mensharapov, Nataliya A. Ivanova, Dmitry D. Spasov, Matvey V. Sinyakov, Sergey A. Grigoriev, Vladimir N. Fateev. *Experimental study of the electrochemical hydrogen pump based on proton exchange membrane for the application in fusion fuel cycle*. Pages 744-751.

An electrochemical hydrogen pump (EHP) can be used in the fuel cycle of fusion devices for purifying (separating) and compressing fuel (a mixture of hydrogen isotopes). One of the distinguishing features of the fuel cycle of fusion devices is a relatively narrow range of operating pressures of the fuel mixture from high vacuum (~1–10 Pa) to several atmospheres (2–3·105 Pa), and in most of the fuel cycle systems, especially in transmission systems (like gas lines), the pressure shall not exceed atmospheric. In this study, the possibility of using EHP with a proton exchange membrane (PEM) in the fuel cycle of fusion devices in the pressure range of 0.01 – 0.30 MPa and temperatures of 20 – 70 °C was considered, and i-V curves were obtained. A regression analysis of the i-V curves was carried out. The temperature dependence of limiting current and resistance of EHP cell was obtained as follows: lnilim=−1140±1001T+(3.0±0.3) and lnρ=1780±2801T+(6.5±1.1). It is shown that there is no dependence of these parameters on pressure. The EHP cell productive capacity was determined in the studied ranges of pressure and temperature as follows: lni2F=−0.0119×T−4.2×Ecell0.05+Ecell+20.4. The results obtained allow one to predict the performance of the EHP device under conditions of subatmospheric hydrogen pressure at the anode and to select the most effective operating parameters of the EHP.

- **Keywords:** Electrochemical hydrogen pump; Hydrogen compression; Hydrogen purification; Proton exchange membrane; Fusion fuel cycle; Subatmospheric pressure

Di Chen, Chengqing Wu, Jun Li. *Assessment of modeling methods for predicting load resulting from hydrogen-air detonation*. Pages 752-765.

As hydrogen becomes an increasingly vital component in the transition toward a sustainable energy system, its flammable and detonable properties necessitate a comprehensive understanding of its explosive characteristics. This study evaluated the accuracy and computational efficiency of an innovative numerical approach that integrates CESE compressible CFD solver, chemistry reaction model, and structural FEM solver within LS-DYNA to predict hydrogen detonation loads. Comparisons were made with the commonly used energy equivalent methods, i.e., the TNT equivalent method, and the high-pressure volume method, which utilizes multi-material ALE techniques. Hydrogen detonation test results from open-air space, open-air space with a blast wall, and semi-confined space were compared against numerical simulations. The results revealed that, for scaled distance exceeding 0.79 m/kg1/3, all three methods accurately

predicted the peak overpressure. The TNT equivalent method exhibited an unexpectedly high energy efficiency factor exceeding 0.51, significantly surpassing the recommended range of 0.01–0.1 for typical vapor cloud accidents. The CESE-chemistry coupling method exceled in capturing overpressure duration and structural response due to its consideration of chemical kinetics. As the scaled distance reduced to 0.37 m/kg1/3, the CESE-chemistry coupling method maintained its proficiency in modelling pressure waves, while the TNT equivalent method overestimated peak pressure by 494%. Conversely, the high-pressure volume method underestimated the peak pressures within or near the H2-air cloud. Nevertheless, the CESE-chemistry coupling method required significantly higher computational costs, with 15–20 times more computational time compared to the other two methods, and 60–70% of the total computation time was spent solving chemical kinetics. It is concluded from the current study that for scenarios involving close scaled distances (less than 0.37 m/kg1/3) or where the structure locates inside or near the gas cloud, the CESE-chemistry coupling method may be preferred despite its higher computational demands. Conversely, for simulations prioritizing computational efficiency and larger scaled distances, the TNT equivalent method or high-pressure volume method is recommended. These findings offer guidelines for researchers and engineering professionals engaged in assessing and mitigating risks associated with hydrogen explosion accidents in the pursuit of safe and sustainable hydrogen utilization.

- **Keywords:** Hydrogen detonation; Load prediction; Modelling; Fluid-chemistry-structural coupling; Multi-material ALE

Wenxin Wang, Haiyang Cheng, Qing Zhao, Yangyang Wang, Xin Li, Zhaoyou Zhu, Yinglong Wang, Fang Wang, Peizhe Cui. *Economic, environmental, exergy (3E) evaluations of recovering n-propyl acetate and n-propanol from wastewater via distillation coupled pervaporation*. Pages 766-777.

This work investigates an efficient and sustainable process for recovering n-propyl acetate and n-propanol from wastewater via extractive distillation coupled with pervaporation (PV). The selection of potential extractants is based on the equilibrium data between the system and the extractants in vapor-liquid phase. For the ternary extractive distillation process, we optimize it using the Non-Dominated Sorting Genetic Algorithm II with the objectives of minimizing the total annual cost and gas emissions. The PV model is integrated with the distillation process to enhance solvent recovery, while an energy-efficient scheme combined with heat integration technology and heat pump improves separation efficiency. Economic, environmental and exergy analyses are conducted to evaluate feasibility, revealing that coupling extractive distillation with PV enhances economic and environmental benefits compared to basic processes. The combination of heat pump assisted heat integration technology further improves the economy performance, environmental protection and thermodynamic efficiency, and the process selection needs to be balanced according to the actual industry.

- **Keywords:** Extractive distillation; Pervaporation; Multi-Objective Optimization; Heat integration

Zhiyu Fang, Lang Liu, Xiaoyan Zhang, Keming Han, Jingyu Wang, Mengbo Zhu, Weiji Sun, Wei He, Yuheng Gao. *Carbonation curing of modified magnesium-coal based solid waste backfill material for CO2 sequestration*. Pages 778-788.

CO2 sequestration is an effective method for dealing with the global climate crisis, and carbonation curing is considered an effective method of sequestering CO2 and improving the mechanical properties of cement-based materials (CBM). Regarding modified magnesium-coal based solid waste backfill material (MB), to explore its carbonation

curing performance and CO2 sequestration capacity, its uniaxial compression strength (UCS), carbonation depth, microstructure, CO2 transport performance, CO2 uptake capacity, and carbonation efficiency are analyzed and characterized using UCS tests, thermogravimetric analysis (TGA), X-ray diffraction (XRD), and nuclear magnetic resonance (NMR) analysis. The results show that the early UCS of the MB is significantly improved by carbonation curing. The UCS at 7 days is 10.91 times higher than that of the MB without carbonation curing, and the UCS increases as the concentration and modified magnesium slag-based cementitious material (MC) content increase. Carbonation curing makes the microstructure of the MB significantly denser and reduces the porosity, pore diameter, and permeability. The formation of carbonated products such as calcium carbonate and hydration products makes the microstructure more compact, which is the main reason for the rapid increase in the early UCS of the MB. The maximum CO2 uptake capacity of the MB through carbonation curing is 14.3%, and the carbonation efficiency is up to 92.2%. Therefore, carbonation curing of MB has broad application potential in improving the UCS and sequestering CO2.

- **Keywords:** Carbonation curing; Solid waste backfill material; UCS; Microstructure; CO2 sequestration

Mengjin Zhou, Ruoyu Hu, Yanan Li, Ranran Wei, Zhaoyou Zhu, Yinglong Wang, Jingwei Yang, Jianguang Qi, Chaoyue Sun, Xinling Zhao, Peizhe Cui. *Separation process and mechanism of cyclohexane/ethanol system using deep eutectic solvents based on betaine and choline chloride*. Pages 789-799.

The efficient separation of azeotropes is of great significance for the effective recovery and utilization of chemical raw materials and environmental protection. This study investigated the separation efficiency and mechanism of deep eutectic solvents (DESs) with different combinations and ratios of hydrogen bond acceptors (HBA) and hydrogen bond donors (HBD) for cyclohexane/ethanol azeotropic systems. Through vapor-liquid phase equilibrium experiments, the effects of different DESs and different HBD: HBA molar ratios as solvents on the phase behavior of cyclohexane/ethanol azeotropic system were studied, and different combinations and molar ratios of DESs with the best separation performance were obtained. The effective separation of azeotropes by DESs is primarily due to the stronger molecular surface electrostatic potential of ethanol compared to that of cyclohexane, which results in a stronger interaction between the DESs and ethanol. Finally, through process simulations, a cyclohexane/ethanol extractive distillation separation process using a DES as the main solvent was established. The results showed that the separation effect of DESs increased with the increase of the interaction force between DESs and ethanol, achieving efficient recovery of chemical raw materials. This study established a safe and efficient separation process using DESs, which is of great significance for environmental protection and the development of safety processes.

- **Keywords:** Deep eutectic solvents; Quantum chemical calculation; Extractive distillation; Azeotrope separation

Rahul Mishra, Aman Kumar, Ekta Singh, Archana Kumari, Sunil Kumar. *Synthesis of graphene oxide from biomass waste: Characterization and volatile organic compounds removal*. Pages 800-807.

This research study focuses on analyzing the effects of graphene oxide (GO) synthesized from subabul, pine, and copperpod biomass waste for the adsorption of volatile organic compounds (VOCs). Five different VOCs i.e., benzene, xylene, carbon tetrachloride, n-hexane, and toluene were utilized for the sorption experiment. A modified Hummers process was carried out for the successful GO production from biomass waste and the

obtained GO was confirmed using SEM, Raman spectroscopy, FTIR, and XRD. The existence of 2D-mode and G-mode in Raman spectroscopy as well as O-H and C=O groups in the FTIR confirmed the GO synthesis. The sorption efficiency of SGO, PGO, and CGO for different VOCs was in the range 82–146, 74–144, and 126–166 mg g−1, respectively. The sorption of VOCs was also affected by feedstock type, contact time, and dose of GO. The sorption efficiency of GO increased with a long contact time and higher surface area. Furthermore, for statistical analysis, ANOVA was used. For the kinetics of VOCs sorption, the pseudo-second-order model was utilized, which well fitted with the findings of this research study. The excellent sorption performance of GO produced from biomass waste made it a potential adsorbent for the sorption of VOCs.

- **Keywords:** Graphene oxide; Biomass waste; Hummer's method; Volatile organic compound; Sorption

Zhongjie Fei, Su Zhanguo, N.Bharath Kumar, Pradeep Kumar Singh, Zainab A. Farhan, Mahidzal Dahari, Haitao Lin, H. Elhosiny Ali, Souhail Mohamed Bouzgarrou. *Clean and sustainable power/fresh water/hot air production scheme based on solid oxide fuel cell feed by apricot stone biomass: A multi-attribute optimization*. Pages 808-826.

Developing novel and low-emission multi-generation systems is attracting considerable critical attention. In this regard, a novel tri-generation of power, fresh water and hot air has been developed in this study based on solid oxide fuel cell. Power has been generated by a solid oxide fuel cell, a gas turbine cycle and a super-critical carbon dioxide Brayton cycle. An air flow has been heated in a heat exchanger and fresh water has been produced through a desalination unit. Super-critical carbon dioxide Brayton cycle, heat exchanger of hot air and desalination unit have been all triggered by a co-combusted gas of apricot stone and synthesis gases of solid oxide fuel cell. Analysis of variance has been utilized to identify the significant influences on power production, fresh water, hot air, emission effect of system and system efficiency. Multi-objective optimization has showed that apricot stone of 200 kg/h, fuel utilization of 0.77, current density of 9697 A/m2 and pressure ratio of 3 in gas turbine system are the optimum conditions. The system has produced 2.10 MW of power, 837 g/h of fresh water and 57 m3/h of hot air with an emission effect of 2069 kg/MW.h and an efficiency of 43.5%.

- **Keywords:** Tri-generation system; Biomass energy; Solid oxide fuel cell, Multi-attribute optimization

Chi-Wen Lin, Jin-Shuo Liu, Shu-Hui Liu. *Promoting electricity generated from sediment-based microbial fuel cells and remediation of copper-containing sediments using plant radial oxygen loss and root exudates*. Pages 827-836.

This study uses root exudates and radial oxygen loss (ROL) produced by plants to increase the amount of power produced by sediment microbial fuel cells (SMFCs) and improve copper removal. Among the three plants tested, which are commonly found in wetlands, Ipomoea aquatica produces the highest yield of root exudates and ROL, with respective values of 8.54 mg/(g·d) and 2.1 μmol/(g·h) at 50-mg/L Cu inhibition. The maximum power density of an SMFC with 450 mg/kg of copper-containing sediment and Ipomoea aquatica planted at the anode is 58.4 mW/m3, which is three times greater than that of an SMFC with Ipomoea aquatica planted at the cathode. This demonstrates that plant root exudates provide anodic microorganisms with easily decomposed organic matter, which increases the amount of power. The presence of a bioelectrochemical process is demonstrated by the presence of Cu(II) reduction deposits on the cathode surface. According to the findings, planting Ipomoea aquatica at the anode produces more electricity and removes slightly less copper than planting it at the cathode. It is

concluded that planting Ipomoea aquatica at the anode is more effective than planting it at the cathode.

- **Keywords:** Root exudates; Radial oxygen loss; Copper inhibition; Ipomoea aquatica; Plant growing position

Zhiheng Xia, Zhao-Dong Xu, Hongfang Lu, Haoyan Peng, Zicong Xie, Yankun Jia, Hui Sun. *Leakage analysis and prediction model of underground high-pressure natural gas pipeline considering box culvert protection*. Pages 837-855.

Buried gas pipelines frequently experience failures as a consequence of adverse factors. The studies of gas leakage diffusion behavior and prediction of hazardous areas following pipeline failure hold profound significance in mitigating the risk of accidents. This paper exemplifies a specific segment of long-distance transportation gas pipeline in the "West-to-East Gas Transmission" project, employing the Soave-Redlich-Kwong (SRK) equation of state (EOS) to develop a numerical model for high-pressure gas leakage and diffusion, while considering box culvert protection. The characteristics of gas leakage diffusion and the effects of pressure, leakage diameter, and soil type on gas diffusion are presented. Furthermore, the prediction models for leakage rate, fastest hazardous time (FHT), fastest hazardous distance (FHD), and lateral hazardous distance (LHD) are introduced. The results show that the pressure and velocity at the beginning of the leakage manifest an annular diffusion centered on the leakage hole, stabilizing within 300 s. The gas primarily diffuses along the horizontal direction within the box culvert, and the peaks of gas concentration at the surface are situated at a distance of 2.35 m on either side of the pipeline. Variations in pressure and leakage diameter influence the gas concentration but do not alter the locations of the concentration peaks observed at the surface. The greater the viscous and inertial resistance of the soil, the shorter the overall diffusion distance becomes. However, backfilling the loam within the box culvert significantly elevates the concentration of gas that leaks to the surface. The leakage rate, FHT, FHD, and LHD can be well calculated by the prediction models proposed in this study.

- **Keywords:** High-pressure; Natural gas; Buried pipeline; Leakage diffusion; Hazardous area; Prediction model

Zihao Xiu, Zhenyi Liu, Pengliang Li, Mingzhi Li, Yao Zhao, Tao Fan, Jie Yuan. *Progress of research on the effect of non-uniform premixing on hydrogen and methane explosion characteristics*. Pages 856-867.

This study attempted to systematically understand the research results on the explosion disaster effects of premixed hydrogen and methane gas driven by concentration. Based on the effect of obstacles on the explosion characteristics of non-uniform premixed gases, the experimental approach of non-uniform concentration distribution was comprehensively determined, and the experimental and numerical simulation results of the influence of non-uniform distribution on flame acceleration and deflagration to the detonation process were discussed. The results showed that the effects of non-uniform premixing on the hydrogen and methane deflagration characteristics were different in the unobstructed space. For hydrogen, the smooth pipe exhibited stronger flame acceleration and earlier deflagration to detonation, whereas for methane, the presence of concentration gradients did not promote flame acceleration or an overpressure rise. The presence of a critical value between the average fuel concentration and the concentration gradient in an obstructed space can result in flame acceleration or slowdown; however, owing to the limitations of the experimental method and equipment, the current results did not yield a more accurate critical value. Consequently, a new experimental device was proposed to investigate combustible gas deflagration driven by the concentration gradient, which provided a basis for further experiments on the influence of the

concentration gradient interval on the deflagration characteristics of the premixed gas in the later stage. This review aimed to provide new research ideas and methods for studying the deflagration characteristics of combustible gases under nonuniform premixed conditions.

- **Keywords:** Non-uniform; Hydrogen and methane; Deflagration characteristics; Obstacles

Joel Sansana, Ricardo Rendall, Mark N. Joswiak, Ivan Castillo, Gloria Miller, Leo H. Chiang, Marco S. Reis. *A functional data-driven approach to monitor and analyze equipment degradation in multiproduct batch processes.* Pages 868-882.

Equipment degradation is ubiquitous in the Chemical Process Industry (CPI), causing significant losses in efficiency, controllability, and plant economy, as well as an increased environmental fingerprint and additional operational safety risks. The case of fouling in heat exchangers, in particular, is well-known and pervasive but still hard to cope with, given the complexity of the underlying mechanisms and the difficulty of assessing its extension in real-time. This problem becomes even more complex in batch processes producing different products, where multiple recipes are used, bringing additional variability and new challenges to the analysis. In this work, we propose a functional data-driven approach for streamlining the analysis and monitoring of the progression of fouling taking place in heat exchangers in multiproduct batch processes. With the approach developed and presented in this paper, process analysis can be efficiently conducted by integrating historical data with engineering knowledge. Furthermore, a surrogate measure of fouling extension in heat exchangers is proposed, that can be readily implemented as an equipment health indicator (EHI) leading to a safer operation of the heat exchanger.

- **Keywords:** Batch process; Functional data analysis; Fouling diagnostics; Heat exchanger; Multiproduct

Bo Liu, Xiaoguang Ying, Yilan Zhang, Jiaqi Lv, Bo Yang, Xiao Li, Haiqiang Chen, Jiangquan Liu. *Polyurethane nanofiber membranes immobilized with Bacillus altitudinis LS-1 for bioremediation of diesel-contaminated wastewater*. Pages 883-892.

Oil pollution from the petroleum industry is a growing problem, especially in terms of the harm it causes to the aquatic environment, which puts humans and other aquatic life in grave danger. As immobilized carriers for the removal of diesel, thermoplastic polyurethane (TPU) nanofiber membranes and co-blended nano-hydroxyapatite modified thermoplastic polyurethane (TPU/nHA) nanofiber membranes are reasonably priced, non-toxic, and non-polluting. The adhesion and colonization of the bacterial cells to these carriers were studied using scanning electron microscopy (SEM). Gas chromatography was used to measure the bioremediation effectiveness, and the results after 3 days of remediation revealed a substantial improvement in the removal of hydrocarbons by immobilization compared to free bacteria. With an initial concentration of 3 g/L diesel, the TPU/1.5HA-bacteria system enhanced the removal of diesel the most (20.64 ± 0.40%), followed by TPU/1HA-bacteria (17.49 ± 0.08%), TPU/0.5HA-bacteria (11.97 ± 0.40%), and TPU-bacteria (4.69 ± 0.13%), in that order. Within three days, these scaffolders had completely absorbed the spilled diesel. There haven't been any studies done yet on the removal of diesel using various carriers loaded with Bacillus altitudinis LS-1. This study demonstrated that TPU-based electrostatic spinning films can be used as bio-carriers for hydrocarbon-degrading bacteria, enhancing the bioremediation of oil-contaminated water.

- **Keywords:** Bioremediation; Immobilized carriers; Diesel; Oil-adsorbing membranes; Bacillus altitudinis

Chengcai Wei, Zhenmin Luo, Yingying Yu, Tao Wang, Yong Yang, Haitao Li, Shoutong Diao, Jingyu Cui, Minggao Yu. *Experimental and kinetic investigation of the explosive behavior and free radical spectroscopic characteristics of hydrogen/propane mixed gas*. Pages 893-906.

A detailed investigation of the explosion mechanism of hydrogen (H2) - propane (C3H8) mixture gas is the prerequisite for effective prevention of its explosion. This study delved into the explosion pressure and the spectral intensity of free radicals within the H2-C3H8 mixture, conducting a comprehensive investigation of reaction kinetics to elucidate reaction rates, elementary reaction sensitivity, and reaction path. Our findings unveiled a relationship between hydrogen augmentation and heightened explosion pressure, particularly when the hydrogen mixing ratio exceeded 80.0%, and the explosion index reached to St3 level, thereby indicating an exceeding safety risk. Moreover, a discernible augmentation was observed in the spectral intensities of H•, OH•, and O• radicals in tandem with an increased hydrogen mixing ratio. Notably, a linear correlation emerged between the explosion pressure and the spectral intensities of these free radicals. R1: H•+O2 =O•+OH• was the most important reaction step. As the ignition starts, H2 burns prior to C3H8, giving rise to the generation of H• radicals. These H• radicals, in turn, actively participate in the dehydrogenation of C3H8, effectively catalyzing the overall chemical reaction. These results can provide potent scientific support and guidance for the prevention and management of H2-C3H8 explosions.

- **Keywords:** Hydrogen; Propane; Explosion risk; Free radical spectrum; Reaction kinetics

Aravindan Santhan, Kuo Yuan Hwa, Ravikumar Murugan. *Rational construction of 2D heterostructures: Niobium carbide entangled rGO aerogel for the detection of para nitroaniline isomer in environmental water samples*. Pages 907-922.

4-Nitroaniline (4-NTA) is considered to be an environmental pollutant that is extremely hazardous to the ecosystem which is found in an inclusive range of industrial chemicals that includes dyes, pigments, fungicides, and pesticides. When 4-NTA occurs in water it seems to be highly carcinogenic to human beings. In consequence, there's a critical need for monitoring and identifying ecologically highly hazardous 4-NTA, specifically in water samples. Herein, the design of a novel niobium carbide/reduced graphene oxide aerogel (NC/rGO-A) was prepared to perform effective electrochemical recognition of 4-NTA in environmental water samples. The specific features of rGO-A with high porosity, and higher electrical conductivity, when coordinated with metal carbide, will sufficiently provide higher active sites resulting in excellent performances. Various methods of investigation have been employed to identify the physical and chemical characteristics. The fabricated NC/rGO-A sample over the screen-printed carbon electrode (SPCE) has been subjected to sensing investigation with a wide linear range of 0.039−1602 μM with good sensitivity 27.96 μA μM−1 cm2, the limit of detection at 4.6 nM for 4-NTA detection. Furthermore, the designed 4-NTA sensing exhibited excellent anti-interference, reproducibility, repeatability, and stability. The as-developed sensor's electrochemical analysis outcomes indicate the superior performance inherent in the developed composites.

- **Keywords:** Environmental water pollutant; 4-Nitroaniline; DPV detection; Niobium carbide; RGO-aerogel

Xiang Zheng, Danyang Dai, Helin Hua, Dawei Yu, Rong Cheng, Libing Zheng. *Aging behavior and mechanism of polyvinylidene fluoride membrane by intensified UV irradiation and NaOCl: A comparative study*. Pages 923-934.

Membrane technology plays a critical role in solving worldwide water scarcity and security issues. However, membrane aging causes deterioration or complete failure of membrane performance. In this work, polyvinylidene fluoride (PVDF) membrane aging induced by ultraviolet (UV) and NaOCl were investigated and compared. The skin layer was completely destroyed in 2d by UV irradiation under a dry state, which further caused deformation in the sublayer and pore shrinkage. The water layer on the membrane surface protected the skin layer from damage by UV till 8d under the wet state. NaOCl had a moderate influence, the flux was firstly decreased as the hydrophobicity of the membrane increased, and then increased due to pore enlargement. Membrane aging also resulted in a lower virus rejection, which highlighted the biosafety concern in membrane-based wastewater treatment. Infrared and two-dimensional correlation spectroscopy confirmed that the hydrophilic additive was first oxidated in both processes. β-PVDF segment changed before α-PVDF under UV, during which the CC bond was formed by the dehydrofluorination reaction. But the α-PVDF segment was attacked firstly by NaOCl, the radical reaction occurred both at CH2-CF2 and CH=CF segments. This work studied two aging patterns in the membrane lifecycle and demonstrated the aging mechanism, which shed light on membrane development and maintenance in the future.

- **Keywords:** Membrane aging; Ultraviolet irradiation; Chemical cleaning; Membrane lifespan; Dehydrofluorination; PVDF

Bin Zou, Xin Wang, Jiajun Li, Zhenfeng Cheng, Guotao Ye, Wenhao Yang, Liangyuan Qi, Pengfei Jia, Fukai Chu, Zetao Xiao, Lei Song, Zhou Gui, Yuan Hu. *Harmonization of semi-objective ANP with explained CRITIC for quantitative evaluation of fire hazard risks for flame-retardant materials*. Pages 935-944.

The fire hazard assessment of polymers and the effect of flame retardants constitutes the foundation for preventing and managing fire risks to public safety. This study addresses key challenges by considering intrinsic hazards, indicator volatility and correlations, while overcoming subjectivity in weight assignment and the neglect of flame-retardant treatments. Firstly, we initiate two novel steps of Pearson correlation analysis and predefined comparative scales for indicators, which enhance the objectivity, scalability and repeatability of analytic network process (ANP) weights. Secondly, we utilize the CRITIC method to incorporate indicator volatility and correlations, surpassing the limitations of separate calculations and subsequent combinations. The newly developed pure sample normalization method enhances the interpretability and scientific validity of CRITIC weights. Combining the ANP and CRITIC weights using Nash equilibrium theory, the results rectify the underestimated T-5% from 0.72% to 3.64%, reducing the overestimated PCO2, PSP and TSP from 11.98%, 9.62% and 9.59–7.25%, 9.12% and 5.69%, respectively. Finally, the fire hazards value effectively captures the increased fire hazards resulting from specific degraded indicators following flame retardant treatments. The research findings provide a fresh perspective for the safe design of flame-retardant polymers and fire hazard assessment, offering valuable insights for fire risk prevention and management.

- **Keywords:** Fire hazard assessment; Flame retardant; Black phosphorus; Analytic network process; Pure sample normalization; CRITIC

Haoqing Xu, Tao Sun, Songyu Liu, Nan Zhang, Silin Wu, Pengming Jiang, Aizhao Zhou. *Study on the performance of sealing slurry at the bottom of geomembrane composite vertical cut off walls*. Pages 945-958.

At the bottom of the geomembrane cut-off walls, pollutants may seep out through the bottom gap between the geosynthetic membrane and the low-permeability bedrock, contaminating the groundwater and the surrounding environment. Therefore, to address the occurrence of bottom gap seepage, this study adopts a mixture of attapulgite and cement in a certain proportion, mixed and stirred to form a sealing material. This sealing material is used to connect the bedrock and the geosynthetic membrane, thereby creating an efficient composite vertical barrier with special containment capacity. A series of laboratory experiments were conducted to investigate engineering properties of cement-attapulgite sealing slurry, including flow value tests, unconfined compressive strength (UCS) tests, improved flexible wall permeability tests, and bedrock and sealing slurry adhesion tests. The results show that the flow value of the slurry decreases with the increase of attapulgite content, and it increases with the increase of water-cement ratio. The UCS strength increases with the increase of attapulgite content, and it decreases with the increase of water-cement ratio, but the range of change is different. The hydraulic conductivity measured with hexavalent chromium solution as the penetrant is less than 50 % higher than that measured with water as the penetrant, and hexavalent chromium solution has little effect on the hydraulic conductivity of sealing slurry. The bonding performance between sealing slurry and bedrock is satisfactory, and the hydraulic conductivity of bedrock-sealing slurry is less than $1 \times 10-7$ cm/s (28d curing age), it is concluded that use of cement-attapulgite sealing slurry as bonding material between bedrock and geomembrane meets the engineering design requirements.

- **Keywords:** Cement-attapulgite sealing slurry; Flow value; Unconfined compressive strength; Hydraulic conductivity; Bedrock

Yang Liu, Lei Xu, Min Chen. *Green and efficient recovery of valuable metals from waste copper slag via co-modification with CaO and Na2O*. Pages 959-971.

In this work, a novel carbon-free smelting reduction process is proposed to recover valuable metals from molten copper slag, in which secondary aluminum dross is used as the reductant via co-modification with CaO and Na2O additions. The influence of Na2O addition on the metal recovery and slag properties under different CaO/SiO2 ratios was investigated at 1550 °C. The results show that the modifier Na2O not only reduces the melting temperature of the slag, but also inhibits the precipitation of spinel and prevents the polymerization of aluminosilicate units to a certain extent by providing more O2-, which results in a relatively lower slag viscosity. These effects are more significant at the CaO/SiO2 of 0.9. The multiple strengthening mechanisms improve the kinetic conditions for smelting reduction, resulting in optimal results when the Na2O addition reaches 4 wt% at the CaO/SiO2 of 0.9, at which 99.1% of iron and 98.5% of copper in the slag can be recovered as the high-purity alloy. The leaching toxicity of the tailings is 2–3 orders of magnitude lower than the original slag, suggesting that they are clean sources for ceramic production. Furthermore, the assessment of the proposed process indicates that it is technically feasible even without an external energy supply, which indicates that the process is green, efficient, and cost-effective.

- **Keywords:** Waste copper slag; Smelting reduction; Modification; Iron recovery; Green recyclin

Quanquan Wu, Zhenqiang Xing, Jianfang Zhong, Qing Wu, Zhengtong Su, Jianlong Li, Hong Huang, Zhifei Ma, Daishe Wu. *Cleaning performance improvement of a cone filter cartridge using a Venturi nozzle*. Pages 972-980.

To address the problem of the insufficient regeneration of dust filter cartridges, a Venturi nozzle is introduced to improve the cleaning performance. The jet distance, cone height, and compressed air pressure effects on the pulsed-jet pressure distribution were experimentally investigated. Changes in the filtration pressure drop, fallen dust mass, and dust emission were also studied. As the jet distance increased, the pulsed-jet pressure and the total pulsed-jet intensity first increased and then decreased for both cases of common and Venturi nozzles, but the pulsed-jet uniformity increased. In the Venturi nozzle case, the pulsed-jet pressure in the lower section of the cartridge was effectively increased due to the larger induced airflow. As the cone height increased, the pulsed-jet pressure in the lower section of the cartridge decreased and that in the upper section increased for both nozzle cases. The dust filtration-cleaning experiment showed that the Venturi nozzle improved the operation performance of the dust collector.

- **Keywords:** Cone filter cartridge; Venturi nozzle; Peak pressure; Residual pressure drop; Filtration cycle

Li Dai, Dingliang Xu, Aosong Wei, Minjie Shan, Pengcheng Tao, Zhuofan Deng, Jianping Li, Jianqi Chen, Hualin Wang. *Purification of hydrogenated oil by microchannel separation coupling hydrocyclone*. Pages 981-991.

Hydrogenated oils are commonly used as solvents in the petroleum resin industry. The separation of particulate matter from hydrotreating oil is critical to product quality and the service life of the catalyst in the downstream fixed bed. Conventional separation methods, represented by diatomaceous earth filtration, suffer from low separation efficiency, high material consumption, generation of large amounts of hazardous waste, and cumbersome operation. Therefore, a physical method of microchannel separation coupling hydrocyclone was proposed. A 1 m3/h pilot pretreatment device was established to comprehensively evaluate the particle removal in hydrogenated oil. The high separation efficiency and long operation cycle were achieved by a microchannel separator with 0.5–1 mm particle size quartz sand. The single cycle of the microchannel separator was 75 h. The turbidity was decreased by about 64.3%, which was better than that of the traditional separation method (49.9%). The particle removal in hydrogenated oil by microchannel separator was about 75.0%, while the removal of diatomite separator in the same period was only 44.7%. In a 40 m3/h petroleum resin plant based on a microchannel separator, the operating cost and the hazardous waste emissions are reduced by 1,815,000 CNY/year and 208 tons/year, respectively. It is hoped that this study can not only promote the energy-saving and cleaner production of hydrogenated oil but also provide useful guidance for other petrochemical industries.

- **Keywords:** Petroleum resin; Physical separation; Process transformation; Emission reduction

Jialong Liu, Longfei Zhou, Yun Zhang, Tengfei He, Zhirong Wang. *Thermal stability of lithium-ion battery subjected to inhomogeneous aging*. Pages 992-1002.

Aged battery is prone to fire accidents. Thermal stability change of battery subjected to inhomogeneous aging is studied in this manuscript by accelerating rate calorimeter. The results indicate that thermal runaway time decreases for aged batteries. Solid electrolyte interphase and lithium plating suppress and accelerate onset exothermic side reactions.

Transition metal dissolution accelerates positive electrode decomposition and oxygen release. TTR of aged batteries decreases compared to fresh battery. Microscopic changes of negative electrodes for batteries cycled at high and low temperature are inhomogeneous. Tonset for batteries cycled at low temperature decreases as lithium plating covers all of the negative electrode surface. Tonset for batteries cycled at high temperature and with 100% state of charge (SOC) increases. This is the same to battery stored at high temperature. Local lithium plating affects thermal stability of battery with 100% SOC less. However, Tonset for batteries with SOC lower than 50% SOC and subjected to local lithium plating decreases compared to fresh battery. Local lithium plating accelerates onset exothermic side reactions for battery with SOC lower than 50% SOC. The results of this manuscript are important to thermal runaway prevention for batteries in their whole operation life.

- **Keywords:** Aged battery safety; Thermal stability; Local lithium plating; Inhomogeneous aging

Mevlut Uyan, Ela Ertunç. *GIS-based optimal site selection of the biogas facility installation using the Best-Worst Method*. Pages 1003-1011.

Renewable energy is currently a part of the energy supply. Türkiye, which has a significant potential in terms of renewable energy, offers various supports for biogas energy production. Biogas plants should be established at appropriate locations based on their legal requirements and efficiency. In this study, the application of the Best Worst Method (BWM) and Geographic Information System (GIS) integration for determining suitable locations for biogas plant installation in Türkiye, is presented. First, a suitable region for facilities was determined in a nationwide study. Subsequently, six criteria were determined for the selection of appropriate locations in line with the opinions of experts in this region. By overlay analysis using a GIS software, six criteria were combined using weight values and a site selection suitability map was generated. This map was divided into four classes as unsuitable, low suitability, moderate suitability and high suitability. When the spatial distribution of the suitable areas for the establishment of a biogas facility was examined, it was determined that the high suitability areas were 19931 ha (7.17%), the moderate suitability areas were 22805 ha (8.20%), the low suitability areas were 18300 ha (6.58%), and the unsuitable areas were 2786 ha (1%). The restricted area in this study were 219519 ha (77.04%). In this study, the site selection process was carefully planned and local factors, regulations and environmental impacts were taken into consideration. Correct site selection for biogas plants ensures efficient, environmentally friendly and economically sustainable operation of the plant.

- **Keywords:** Renewable energy; Site selection; Geographical information systems; Multi-criteria decision making

Hamed Mohammaddoost, Maryam Asemani, Ahmad Azari, Behzad Vaferi. *Investigation of methane and ethane diffusivity in the glass reinforced epoxy composite: Experimental and simulation*. Pages 1012-1022.

New polymeric pipes have been used to overcome difficulties created by metal pipes in gas transmission lines such as corrosion and leakage. In this work, diffusion and solubility cells are designed to determine the diffusivity and possible leakage of methane and ethane gases in the glass-reinforced epoxy (GRE) composite. A composite sample with a diameter of 5.95 mm and thickness of 1.40 mm to determine the diffusivity and a composite powder to estimate the gas solubility are used. The experiments are done under temperatures varied from 25 to 40 ℃ and a pressure of 20 bar. The results show that the diffusivity of both gases increases with increasing temperature; while gas solubility decreases. The highest diffusion coefficient of methane and ethane are observed at $8.23 \times 10{-}11$ and $7.94 \times 10{-}11$ m2/s at 40 ℃, respectively. Moreover, novel correlations for estimating gas diffusion coefficient and mass flow rate in terms of

temperature are developed based on the experimental data with the correlation coefficients (R2) of 0.98 and 1 and the average relative error percent (AREP) less than 4.5% and 0.5%, respectively. Interestingly, CFD (Computational fluid dynamics) results show a good consistency with experimental data for gas concentration profiles through the composite with AREP ranges of 1.95–15.78%.

- **Keywords:** Diffusion coefficient; Ethane; Glass reinforced epoxy; Methane; Solubility

Afraa H. Kamel, Raed A. Al-Juboori, Muayad al-shaeli, Bradley Ladewig, Salah S. Ibrahim, Qusay F. Alsalhy. *Potential application of hybrid forward osmosis – Membrane distillation (FO-MD) system for various water treatment processes.* Pages 1023-1052.

Different membrane processes have been used to address water scarcity issues. Among them, membrane distillation (MD) is a promising technology due to its capacity to treat hypersaline water. Forward osmosis (FO) is another innovative technology that has the advantage of low operational energy. A hybrid system of these two technologies has proven to be an effective technique for the water treatment industry particularly for water reclamation and resource recovery. Understanding the fundamentals of this amalgamation and the challenges that brings with it is an important topic for the scientific and research community. This work presents a detailed review of the FO-MD systems enriched with the recent advances in this system. The opportunities and challenges for the individual technologies and the system overall were critically addressed. Successful pilot designs for the hybrid system were illustrated. Mathematical modeling for the water transfer in the hybrid system was also elaborated to identify the key points and boundaries of the processes. It is apparent that the inherent low energy conversion in MD and the need for draw solution regeneration are the prominent challenges of this system. Another important aspect to be highlighted is that the water transfer balance between MD and FO is the key requirement for a stable and successful operation. The use of alternative energy is possible but it is only feasible in specific cases such as the existence of seawater and wastewater facilities in a proximity or the case of produced water that contains geothermal heat. Implementing heat recovery in the MD stage, using functionalized particles as a source of osmolarity in the draw solution, and developing membrane materials with unique characteristics such as omniphobic and Janus MD membranes are effective strategies that have just recently shown to improve the systems economics and such strategies should be explored further.

- **Keywords:** Forward osmosis (FO); Membrane distillation (MD); Hybrid FO-MD systems; Fouling; Wetting; Energy; Pilot system

Husnain Ali, Zheng Zhang, Furong Gao. *Multiscale monitoring of industrial chemical process using wavelet-entropy aided machine learning approach*. Pages 1053-1075.

In recent decades, machine learning (ML) techniques have been effectively applied for industrial process monitoring to assure safety and high-quality yield. Traditional process fault detection, identification, and diagnosis (FDI&D) approaches are insufficiently smart to address the modern complex challenges of real-time industrial chemical processes. The detection and diagnostic resolution of the traditional monitoring approach are less robust, inefficient, and produce the wrong interpretation of actual fault information. These approaches are based on a single-scale fault illustration and cannot effectively address multiple fault depiction roots. This study introduces a novel ML-aided methodological framework for industrial and manufacturing monitoring systems. The proposed ML framework is developed using Principal component analysis (PCA), Shannon information entropy (IE), wavelet transformation (WT), and signed directed graph (SDG).

It includes fault detection, identification, and diagnostic propagation root-path interpretation to address the safety challenges of modern, real-time industrial chemical processes. The proposed methodological framework is validated using the Tennessee Eastman process (TEP) benchmark to highlight their performance and efficiency. The results of this study determined that the new proposed approach is more efficient in terms of accuracy, robustness, and actual propagation root cause than traditional techniques. It has a high fault detection rate (FDR), low fault alarm rate (FAR) that identifies and recognizes the actual faulty-correlated variables to establish the SDG model framework for determining the actual diagnostic propagation root path. It initially enables operators to react to unusual incidents, ensuring industrial safety, minimizing economic loss, and avoiding disasters.

- **Keywords:** Machine Learning (ML); Process safety; Process monitoring; Fault detection; Identification; And diagnosis (FDI&D); Robust propagation root cause; Tennessee Eastman process (TEP) benchmark

Andres Gonzalez-Cortes, Damien Burlet-Vienney, Yuvin Chinniah, Abdallah Ben Mosbah, Ali Bahloul, Capucine Ouellet. *Development of a context-specific knowledge base for Inherently Safer Design (ISD) in confined spaces: A resource for designers and end users*. Pages 1076-1093.

Confined space work is an important activity in various industries and a significant cause of workplace fatalities worldwide. Accidents and fatalities persist despite international standards, regulations, and efforts to improve safety in confined spaces. To address this issue, it is crucial to understand and disseminate knowledge on accident prevention strategies for confined spaces, to raise awareness among safety practitioners, and to harmonize communication between designers and end-users to anticipate OHS risks throughout a structure's lifecycle. Besides, confined spaces are unique and context-dependent, which affects the flexibility of their design and modifications. This paper introduces a Confined Space Permanent Collective Protection (CSPCP) knowledge base as a set of design-oriented principles and sub-principles that can be integrated into confined spaces to protect workers. It incorporates data from legislative and normative safety management frameworks, Inherently Safer Design (ISD) principles, literature-based solutions, expert knowledge, and contextual guidance on 112 CSPCP solutions based on the analysis of 19 case studies. This guidance is finally presented as a relational database, considering input from experts and client-side designers to understand the advantages and limitations of CSPCP for retrofitting confined spaces or designing and manufacturing new ones. Moreover, it provides owners, designers, and safety specialists access through flexible queries to help them balance safety, profitability, and investment.

- **Keywords:** Confined spaces; Risk reduction; Inherently safer design; Accident prevention, Occupational health and safety; Knowledge base

Qingyuan Lei, Kanggen Zhou, Xuekai Zhang, Zairong Qiu, Changhong Peng, Dewen He, Wei Chen. *Recycling of spent LiNixCoyMn1−x-yO2 batteries by a glucose reduction-acid leaching approach: Performance and mechanism*. Pages 1094-1103.

Recycling of valuable elements from spent lithium-ion batteries (LIBs) is of critical significance for both economic benefits and environmental sustainability by preventing potential safety hazards and reducing environmental pollution associated with improper disposal. In this study, a glucose reduction-acid leaching approach was proposed to recover valuable metals from spent LiNixCoyMn1−x-yO2. Under the optimized extraction conditions, 99.54% Li, 99.84% Ni, 99.58% Co, and 99.1% Mn were leached out. The kinetic analysis of the glucose reduction-acid leaching process revealed that the reaction

rate was controlled by internal diffusion of valuable metals. The oxidation derivatives of glucose were mainly C6H12O7, C6H10O7, C5H10O6, C4H8O5 and C4H6O6. Through the reductive leaching process, high-valence Ni(III), Co(III), and Mn(IV) metals were reduced to the low-valence state by glucose, allowing for their fast leaching, while glucose was oxidized and decomposed into smaller molecular weight organics. The findings of this study may provide a new strategy for the effective recovery of valuable metals from spent LIBs.

- **Keywords:** Lithium-ion batteries; Reductive acid leaching; Glucose; Oxidation derivatives

Sidhant Pattanaik, Aryan Shyam Savant, Himani Srivastava, A.K. Jeevanantham, Prakash Ramakrishnan, Nanthagopal Kasianantham, D. Sakthivadivel, Abed Alaswad, Tabbi Awotwee. *Combined mixture process design approach for flexible fuel maps development of ternary blends operated gasoline engine*. Pages 1104-1117.

Alternate means of harnessing energy are currently being researched. However, not all demographics are in a position to switch over to these alternatives while complying with the change in existing infrastructure. The present study aspires to evaluate the effectiveness of ternary fuel blends in existing automotive engines to offer a more flexible mode of operation without demanding any modifications to the existing spark-ignition (SI) engine. It focuses on the compatibility between biofuels and pure gasoline as a flexi-fuel alternative in internal combustion engines (ICE) for improved combustion characteristics. Butanol and Lemon Peel Oil (LPO) are highly competitive renewable biofuels for use in internal combustion engines due to their many advantages. Empirical research is conducted on studying mixtures at different engine speeds and blend concentrations. Accordingly, a combined mixture process design model is developed by virtue of the Design of Experiments (DOEs). ANOVA or analysis of variance method is employed, in addition, to determine the influence of input parameters on output parameters. From the results, it is observed that utilizing pure gasoline or a blend with 90% gasoline produced the least amount of peak cylinder pressure (Pmax) alongside minimum levels of mean gas temperature (MGT), and cumulative heat release rate (CHRR). This indicated a lower efficiency of fuel combustion when using higher proportions of gasoline in the blend. Additionally, engine speed is found to have a significant influence over all the performance parameters where it exhibited an inverse relationship which showed that higher engine speed produced inferior results and vice versa. The desirability matrix yields the most optimal blend, displaying a substantial desirability score of 0.683 running on 50% gasoline, 20% n-butanol, and 30% LPO, at 1523.485 rpm. A comparison between the results of Pmax, CHRR, and MGT between pure gasoline and the optimal blend yields a performance enhancement of 16%, 0.5%, and 6.4%, respectively. Overall, from the research, both butanol and LPO meet the ascribed expectations and are observed to significantly enhance the different combustion parameters. These results can thus be further extrapolated to ascertain the partial replacement of straight gasoline in real-life scenarios with butanol and LPO.

- **Keywords:** Butanol; Combined mixture process design; Design of experiments; ANOVA; Ternary blends; Combustion responses

Taolin Zhu, Meng Qi, Mokun Yin, Jing Dang, Xinhua Zhang, Dongfeng Zhao. *On the hazards of proton exchange membrane (PEM) water electrolysis systems using system theoretic process analysis (STPA)*. Pages 1118-1131.

Green hydrogen energy is environmentally sustainable and critical to achieving a carbon-neutral society. Among several water electrolysis technologies, the proton exchange

membrane water electrolysis (PEMWE) system, when integrated with renewable energy sources (RES), is seen as a promising green hydrogen production method. PEMWE is especially preferred for high-pressure operation, which decreases the energy usage and cost associated with hydrogen compression. However, it also poses significant operational risks, such as component reliability under dynamic operation, potential hydrogen leakage due to overpressure or component failure, possible hydrogen-oxygen mixtures in the system, and other unanticipated operational challenges. To fully understand the PEMWE system's operational risk and facilitate risk management, this study conducts a systematic risk analysis using the System Theoretic Process Analysis (STPA) method, involving component failure, system design, human and organizational factors. Combined with the automated and dynamic nature of the system, salient issues during the dynamic operation of the PEMWE system, such as control reliability, component communication reliability and thermal runaway risk, are identified semi-quantitatively. This research is expected to provide a case for STPA research in the highly automated and socio-technical process industry. The findings are expected to offer valuable insights into the safety and reliability of the PEMWE system, providing engineers with technical guidelines for safer system designs, operations, and risk engineering applications, while delivering systematic strategies for risk management. Consequently, a more reliable PEMWE system could lead to the efficient utilization of fluctuating RES.

- **Keywords:** Hydrogen energy; Proton exchange membrane water electrolysis; System Theoretic Process Analysis (STPA); Hazards identification and mitigation

Ali Rezaei, Abdollah Jamal Sisi, Hassan Zarenezhad, Soheil Aber, Alireza Khataee. *Photo/electrocatalytic microbial fuel cell for simultaneous pollutant degradation and electricity production using g-C3N4 anchored on Ag-mIm*. Pages 1132-1144.

The development of photo/electrocatalysts is an idea to simultaneously enhance power generation and pollutant degradation in a microbial fuel cell (MFC), which may improve its efficiency. Herein, a unique approach was taken to enhance the degradation efficiency of methylene blue (MB) by using a photo-assisted MFC technology with an Ag-2-methyl imidazole (mIm)/g-C3N4 photocathode. Various physicochemical analyses were implemented to confirm the successful synthesis of the prepared samples. From the electrochemical analysis, the high current density (0.1 mA cm2) and the low charge transfer resistance were recorded for Ag-mIm/0.01 g-C3N4 under light irradiation, which is more favorable for pollutants removal. Further investigation of the photo-assisted MFC with Ag-mIm/0.01 g-C3N4 modified cathode revealed the maximum power density of 45.37 mW m2 under the light irradiation, which was 1.8 times higher compared with the dark state. The study demonstrated that the degradation efficiency of MB under light can achieve up to 69%, with an initial concentration of 30 mg L−1, after 72 h. This research suggested a promising process for further usage of MFCs in wastewater treatment.

- **Keywords:** Metal-organic framework; Microbial fuel cell; Photo-cathode; Renewable energy; Degradation mechanism