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Guoxi He, Zhiyuan Tian, Kexi Liao, Jun Shi, Liang Wang. *Numerical investigation on the migration of leaked pollutants after liquid pressurized pipeline leakage regarding oil and gas parallel pipelines situation*. Pages 1-16.

Buried parallel pipelines may cause environmental pollution and explosive accidents after leakage due to corrosion, third-party damage or other factors. Here, an actual oil pipeline in-situ is employed as a prototype to establish a two-dimensional incompressible leakage and diffusion model. The model was applied to analyze the effects of different parameters including pipe diameters, burial depths and flat spacing to other pipelines on the diffusion distance of spilled diesel fuel in porous media. The results show that the existence of natural gas pipeline can change both of the polluted shape and the distance range. The natural gas pipeline can effectively inhibit the diffusion range of diesel with the increase of pipe diameter and the decrease of buried depth. A smaller spacing between parallel transmission pipelines, also results in a reduced horizontal diffusion rang. Meanwhile, the dimensionless formulas are fitted based on the Π theorem regarding diesel diffusion range versus diameter of gas pipeline, buried depth, and spacing between parallel pipelines. This study can develop appropriate protocols for detecting and recovering contaminants from paralleling pipeline.

- **Keywords:** Buried parallel pipelines; Diffusion range; Oil pool formation; Time to ground surface; Π theorem

Jinhan Zhou, Xiaohuang Liu, Xiaojie Liu, Weili Wang, Lingqing Wang. *Assessing agricultural non-point source pollution loads in typical basins of upper Yellow River by incorporating critical impacting factors*. Pages 17-28.

Phosphorus and nitrogen pollutions from agricultural non-point source put heavy burden on water environment. Total nitrogen (TN), total phosphorus (TP) and ammonia nitrogen (NH3-N) are important pollutants in the study of agricultural non-point source pollution. This study presents a technical system that accurately calculated the coefficient of pollutants (TN, NH3-N and TP) entering water to grasp the situation of agricultural non-

point source pollution. The system used for coefficient calculation is based on a main framework of driving factor-transmission factor-infiltration factor-interception factor, incorporating critical impacting factors including rainfall, topography, surface runoff, underground runoff, and interception factors. The coefficient was calculated by selecting typical units and extrapolated to the main stream area of the upper reaches of the Yellow River. Our study provides reference and practical basis for the development and application of coefficient model. It provides enlightenment for the calculation of agricultural non-point source pollutants.

- **Keywords:** Pollution load; Non-point source pollution; Rainfall; Topographic driving; Interception; Calculate

Mustafa Vargün, Ahmet Necati Özsezen, Hüseyin Botsalı, Cenk Sayın. *A study on the impact of fuel injection parameters and boost pressure on combustion characteristics in a diesel engine using alcohol/diesel blends*. Pages 29-41.

Engine researchers focused on alcohol fuels since the invention of diesel engines in the 1900s, and the rise in petrochemical costs in the 1970s triggered this concern. This study investigates the impacts of the injection start timing, pilot injection application, and boost air pressure increase, on combustion and exhaust emissions in a common rail diesel engine fueled with ethanol/butan-2-ol/diesel blends. The lowest combustion noise was obtained in the pilot injection application as 83.8 dB in E15B3. The results indicated that the peak point of cylinder gas pressure rose by more than 5 % in the application of pilot fuel injection and advanced injection timing, compared to conventional engine operating conditions. However, maximum CO2 and NOx were seen in the pilot injection application using FBDF as 5.7 % and 670 ppm, respectively. As alcohol rate increases in fuel blends, the average 1.3 °CA in the ignition delay period was increased, while the total combustion period was shortened more than 6 °CA. This result shows that the combustion reactions of alcohol/diesel fuels occur faster than pure diesel. However, the variation in the ignition delay and total combustion periods of the test fuels considerably reduced with pilot fuel injection application. These results indicates that pilot fuel injection may be applied very controlled according to changing engine conditions. It was calculated in statistical analysis that except for the coefficient variation of the maximum pressure increase rate, the other coefficient variation values were relatively stable and below 3 %. In addition, it was determined that the results of the finite element analysis are proportional to the pressure values obtained experimentally.

- **Keywords:** Biofuels; Diesel engine; Engine parameters; FEA; Combustion; Exhaust emissions

Zeming Xu, Changhui Zhang, Chunhong Zhang, Zhe Chen. *Quantitative evaluation on phosphate adsorption by modified biochar: A meta-analysis*. Pages 42-51.

A great deal of research has indicated that modified biochar has better phosphate adsorption ability compared with unmodified biochar, but some results are contradictory, and a quantitative summary of these studies is still missing, implying high uncertainties of the application of the modified biochar. In this study, the phosphate adsorption ability of modified biochar and the closely related environmental parameters were quantitatively evaluated by meta-analysis. Results indicate that, compared with the unmodified biochar, the phosphate adsorption capacity and removal rate of the modified biochar increased by 451 % and 312 %, respectively; the adsorption isotherm constant-Ⅰ (IC-Ⅰ), adsorption isotherm constant-Ⅱ (IC-Ⅱ) and thermodynamic constants significantly increased by 322 %, 163 % and 163 %, respectively. The phosphate adsorption capacity of biochar pre-modified and post-modified significantly increased by 371 % and 514 %, respectively.

The effects of modification on adsorption rate, rate constant, IC-Ⅰ, IC-Ⅱ and thermodynamic constant were significantly different. The effect of physical modification on the phosphate adsorption capacity of was not significantly. In the chemical modification method, the metal modification shows the highest performance on phosphate adsorption in regardless of adsorption capacity, adsorption rate, isotherm constant and thermodynamic constant. Compared with the biochar from other raw materials, the modified manure biochar (preparation and modification of biochar using animal manure as raw material) showed the largest capacity of phosphate adsorption, with a significant raising of 780 %. The effect size of modified biochar on phosphorate adsorption was correlated with the pyrolysis temperature during biochar production. The modified biochar that was prepared at a higher pyrolysis temperature (>700 °C) with higher mineral content is more helpful in improving the phosphate adsorption capacity. This meta-analysis demonstrates that modified biochar generally enhances the aqueous phosphate adsorption when applied to water by using one modification method or in combination with several methods. These findings provide a scientific basis for developing more reasonable eutrophication control strategies toward widespread adoption of biochar as biomaterials for phosphorus removal from the water ecosystem.

- **Keywords:** Modified biochar; Phosphate; Adsorption capacity; Raw materials; Preparation conditions

Albandary Almahri, Moataz Morad, Meshari M. Aljohani, Nada M. Alatawi, Fawaz A. Saad, Hana M. Abumelha, Mohamed G. El-Desouky, Ashraf A. El-Bindary. *Atrazine reclamation from an aqueous environment using a ruthenium-based metal-organic Framework*. Pages 52-68.

The current research describes the synthesis, characterization, and application of a newly developed metal organic framework grounded on ruthenium (Ru-MOF) for the elimination of hazardous chemicals atrazine (AZ) from water. The zeta potential, N2 adsorption/desorption, SEM, TEM, XPS, and FTIR Spectroscopy were used to analyze the Ru-MOF. Ru-MOF has a high surface area of 1058.62 m2.g−1 and micropores with a pore volume of 0.74 cm3.g−1 were produced by the characterization analyses. Additionally, it was discovered that atrazine adsorption produced good results at pH 4 and an adsorbent mass of 0.8 g per liter of solution. The greatest successful fit with the equilibrium facts was provided by the Langmuir model isothermally and Pseudo-Second-Order kinetically at 298 K, with a maximum adsorption capacity of 382.7 mg.g−1. A spontaneous endothermic process was validated using the thermodynamic characteristics. The results of kinetic investigations, which were fitted to a pseudo-second-order model, displayed that equilibrium was got after 90 min. In terms of adsorption kinetics, the experimental results can be represented by the linear driving force model. Additionally, the projected adsorption data of the model agree with the results of the experiment. Box Behnken design study may also show the ideal circumstances for greater atrazine elimination by Ru-MOF. Hydrophobic, π–π interactions and pore filling processes that take place at the surfaces may be used to govern the adsorption mechanisms. When the adsorption capacity was compared to the literature review, it was determined that the Ru-MOF had the best adsorption capacity out of all the preceding adsorbents. Check the adsorbent's regeneration as it demonstrated good efficiency for five cycles, which was deemed a significant cost-saving benefit.

- **Keywords:** Metal-organic framework; Batch adsorption; Herbicide removal; Atrazine, Box-behnken design

Edson Leonardo Scarpa de Souza, Tomaz Henrique Duarte Chorro, Carlos Roque Duarte Correia. *Thermal analysis of arenediazonium tetrafluoroborate salts: Stability and hazardous evaluation*. Pages 69-81.

Arenediazonium salts represent an important class of aromatic organic compounds widely used as building blocks in academia and industry. Due to the high energy associated with the diazonium group, many of these salts are reported as thermally unstable and/or unsafe to work with. However, most of the tetrafluoroborate arenediazonium salts are fairly stable to handle at room temperature both in solution and when dry. Nevertheless, some of these salts, especially those containing heteroatoms in the aromatic moiety, are problematic for their synthesis, and some are indeed highly unstable. To bring some light on this controversial subject, the thermal stability and potential hazards of the 58 most common arenediazonium tetrafluoroborate salts used by us over the last two decades were evaluated under careful conditions. These results are expected to guide conscious decisions on the use and handling of arenediazonium tetrafluoroborates in organic synthesis.

- **Keywords:** Arenediazonium Salts Stability; Thermoanalysis; Differential Scanning Calorimetry; Yoshida Correlation; Pfizer Correlation

Adel Balali, Mohammad Javad Raji Asadabadi, Mahdi Moghimi. *4E assessment and neural network optimization of a solid oxide fuel cell-based plant with anode and cathode recycling for electricity, freshwater, and hydrogen production*. Pages 95-117.

This study presents a novel hybrid system based on solid oxide fuel cell (SOFC) to produce electricity, heating load, and freshwater. A heat recovery method also provides electricity for hydrogen production through proton exchange membrane (PEM) electrolysis. A parametric study and sensitivity analysis investigated the impact of design parameters on the system outputs. Energy, exergy, economic, and environmental (4E) analyses were conducted. The results obtained from the base system show that the net power, freshwater and hydrogen production are 938.94 kW, 360.45 kg/h, and 11.94 kg/h, respectively. Also, the total exergy efficiency, total cost rate, and CO2 emission index are 51.46%, 53.57 $/h, and 0.075 tons/GJ, respectively. This system is optimized by integrating artificial neural networks with the genetic algorithm based on four objective functions. The optimization results reveal that in scenario a, considering the exergy efficiency and the total cost rate as the objective functions, optimal values are 48.69% and 43.98 $/h, respectively. In scenario b, when the objective functions are freshwater production and the total cost rate, the optimal values reach 731.62 kg/h and 67.42 $/h, respectively. Finally, the optimization outcomes in scenario c show that the hydrogen production and total cost rate reach 9.72 kg/h and 46.11 $/h, respectively.

- **Keywords:** SOFC; Freshwater production; Hydrogen production; 4E analysis; Sensitivity analysis; Machine learning optimization

Carmen M. Sánchez-Arévalo, María Cinta Vincent-Vela, María-José Luján-Facundo, Silvia Álvarez-Blanco. *Ultrafiltration with organic solvents: a review on achieved results, membrane materials and challenges to face. Pages 118-137.*

Among all the available membrane processes, ultrafiltration is one of the most commonly used and industrially adapted. Apart from aqueous filtrations, the ultrafiltration of solvent-based solutions has found various applications. Some of them are the recovery of valuable compounds from agro-food industries (olive oil, wine, etc.) and the separation of solvents during edible oil production. However, the contact of the membrane (especially polymeric membranes) with an organic solvent still brings different challenges regarding

permeate fluxes, rejection values and the long-term stability of the membrane. In this review, the results achieved by research works dealing with organic solvent ultrafiltration have been examined, analyzing the effects of the solvent on the process. Additionally, special attention has been paid to the pre-treatment of the membrane. All the applied strategies to pre-condition the membrane have been reported and discussed here. For the first time, all these relevant data have been formally structured and studied in-depth, aiming to gain more knowledge about organic solvent ultrafiltration.

- **Keywords:** Ultrafiltration; Solvent; Organic solvent ultrafiltration; Ethanol; Membrane

Xiangdong Meng, Lihua Jiang, Qiangling Duan, Shuping Wang, Peiyu Duan, Zesen Wei, Lin Zhang, Zhuangzhuang Jia, Kaiqiang Jin, Qingsong Wang. *Experimental study on exploration of optimum extinguishing agent for 243 Ah lithium iron phosphate battery fires*. Pages 138-151.

Nowadays, an effective and clean extinguishing agent or technology is highly desirable for lithium-ion battery (LIB) fires. Herein, the physicochemical properties and extinguishing effects of various extinguishing agents on 243 Ah lithium iron phosphate (LFP) battery fires are investigated systematically. The extinguishing mechanisms are deeply analyzed and the performance is comprehensively evaluated from the aspects of thermal runaway (TR) and toxicity suppression, cooling and extinguishing efficiency. Compared with HFC-227ea, C6F12O can absorb more heat through vaporization, thereby improving extinguishing and cooling efficiency. The lack of chemical inhibition effect and the tiny droplet size make water mist unable to suppress the high-temperature jet fire, but it has the lowest toxicity and highest cooling efficiency of 54.6%. F-500 and FireIce can improve the extinguishing performance of the water mist by encapsulating and taking hydrocarbon fuel away from the fire zone and inhibiting free radicals in the flame, respectively. 3% F-500 has the extinguishing efficiency of 78.4% and TR efficiency of 64.1%, while maintaining the cooling performance well. In the future, a novel type of fire-extinguishing agent with high heat capacity and latent heat, excellent extinguishing performance, high wettability, low toxicity and insulating properties is expected to be developed for LIB fires.

- **Keywords:** Lithium ion battery safety; Thermal runaway; Extinguishing agent; Fire suppression

Andi Mulkan, Nurin Wahidah Mohd Zulkifli, Husni Husin, Ahmadi, Irvan Dahlan, S. Syafiie. *Development of jackfruit (Artocarpus heterophyllus) peel waste as a new solid catalyst: Biodiesel synthesis, optimization and characterization*. Pages 152-168.

This study aims to develop and convert jackfruit (Artocarpus heterophyllus) peel waste (JPW) into a new solid catalyst suitable for biodiesel synthesis. The calcination process of JPW ash was carried out for 2 h at various temperatures ranging from 500, 600, 700, and 800 °C, and the results showed that ash calcined under 500 °C produced the highest yield of 92.38%. Based on the characterization result, potassium, calcium, and magnesium were significant components in the prepared catalyst. These components are desirable in biodiesel synthesis, making the catalyst a promising candidate for this process. The response surface methodology (RSM) revealed that the optimum conditions for the synthesis process include an oil-methanol molar ratio of 1:9, a catalyst weight of 12% (w/w), a reaction time of 105 min, and a constant temperature of 65 °C, yielding a methyl ester content of 98.88%. The reusability result indicated that the JPW catalyst could be used three times with the highest yield of 93.33%. Moreover, the WCO biodiesel properties were analyzed and found to fulfill ASTM D 6751 requirements. This study

demonstrated that JPW can be successfully employed as a solid catalyst for biodiesel synthesis.

- **Keywords:** Heterogeneous catalyst; Jackfruit peel waste; Optimization; RSM; Transesterification; WCO

Shihang Li, Liyuan Liu, Xiaoyu Tan, Hao Liu, Changgeng Gui, Xingyue Chen, Muze Han, Yihan Lin, Jiang Shao, Liang Yuan, Fubao Zhou. *Effects of filter cartridge wetted before filtration and during filtration on the performance of cartridge dust collector*. Pages 169-176.

A growing number of cartridge dust collectors are used in the underground mining, but the underground wetting state have a grave impact on their performance. In order to study the influence of filter cartridge (FC) wetted before filtration and during filtration on the dust collector, a test system was built. The results showed that the pressure drop (PD) of wetted mechanical filter cartridge (MFC) returned to initial PD after 24 h, and coated filter cartridge (CFC) only need 12 h. The PD of pre-wetted FC rose rapidly while filtrated dusty air. The residual pressure drop (RPD) of pre-wetted FC was high, which heavily reduced the service life of FC. If FC was wetting during filtration of dusty airflow, the PD were minimum when the spray rate was 450 mL/ h, and the PD of MFC was higher than that of CFC.

- **Keywords:** Filter cartridge; Spray rate; Wetting state; Pulse-jet cleaning; Filtration performance

Ragu Sasikumar, Byungki Kim. *Development of boron nitride incorporated molybdenum disulfide nanocomposite as a simultaneous electrochemical transducer for environmentally hazardous ortho and para-nitroaniline isomers in aquatic environments*. Pages 177-186.

Harmful nitroaniline isomers are highly environmentally toxic, their main source being the improper release of industrial waste. These isomers are commonly utilized in various chemical products. The presence of these organic compounds in water and the environment poses a significant carcinogenic risk to humans. Therefore, there is an urgent need to monitor and detect these isomers in aqueous mediums to minimize the potential hazards they pose. To tackle this issue, we have developed an electrocatalyst called boron nitride@molybdenum disulfide nanodisk (BN@MoS2 ND) for the simultaneous detection of o-NA and p-NA in tap, river, and mineral water samples. The synthesized nanodisk was characterized using PXRD, FT-IR, Raman spectra, XPS, and FE-SEM studies. The incorporation of BN with MoS2 as a mediator in the reduction mechanism resulted in excellent electron transfer (Rct = 167.73 Ω) and increased surface area (SBET = 31.606 m2 g−1). The proposed sensor exhibited a good linear range, the limit of detection, and sensitivity toward o-NA and p-NA, under pH-regulated conditions, with values of ca. 0.001–778.88 μM, ca. 0.4 nM, and ca. 20.142 (± 0.002) μA μM−1 cm−2 and ca. 0.001–569.96 μM, ca. 0.6 nM, and ca. 14.371 (±0.002) μA μM−1 cm−2, respectively. Furthermore, the BN@MoS2/SPCE demonstrated good recoveries of ~94–99 % for tap, river, and mineral water samples, thereby confirming its excellent ability to detect harmful nitroaniline isomers in aqueous mediums and the environment.

- **Keywords:** Boron nitride; Environmental pollutant; Electrocatalytic reduction; o-Nitroaniline; p-Nitroaniline

Mehdi Khodadadi, Aminolah Masoumi, Morteza Sadeghi, Ahmad Moheb. Modeling and experimental studies on chemical absorption of ammonia emitted from poultry manure during the drying process by a wet spray scrubber: Optimization by Box-Behnken design. Pages 187-201.

One of the most important environmental worries related to poultry production is ammonia gas emission which is affected by poultry manure moisture. This research was aimed at investigating poultry manure drying in a hot air dryer and its influence on ammonium nitrogen losses to provide an overview of ammonia gas emissions and absorption of emitted ammonia by a spray scrubber. The effect of air temperature (60–80 °C), air relative humidity (8–18 %), manure depth (2–4 cm), and air velocity (2–3 m s−1) were analyzed to optimize the drying process. The optimization of ammonia absorption involved analyzing the effects of absorbent solution temperature (30–50 °C), solution pH (2−4), and nozzle operating pressure (0.2–0.6 Mpa). The Box–Behnken design was applied to optimize these processes. Manure depth was the factor that had the most significant effect on both drying duration and ammonia emission (ammonium nitrogen losses). during the drying process, the ammonium nitrogen losses increased with increasing the manure depth and decreasing the air velocity and air temperature. The optimum ammonium nitrogen was 570,330 mg h lit−1 at an air temperature of 60 °C, air relative humidity of 8.11 %, manure depth of 3.95 cm, and air velocity of 2 m s−1. Both the temperature of the absorbent solution and the solution pH had opposite effects on the ammonia absorption. Increasing nozzle operating pressure increased ammonia absorption. The maximum ammonia absorption was obtained at a solution temperature of 49.2 °C, solution pH of 2, and nozzle operating pressure of 0.58 Mpa. At these conditions, the amount of ammonium sulfate in the absorbent solution was 9.09 g lit−1 and the efficiency of the spray scrubber was 66.79 %. So, we can be sure that ammonia emission from poultry manure and the absorption of emitted ammonia can be controlled by varying the investigated variables.

- **Keywords:** Ammonium nitrogen; Ammonia emission; Box–Behnken design; Drying duration; Environmental concerns

Douglas Hungwe, Satomi Hosokawa, Hao Xu, Lu Ding, Yuki Yamasaki. *Effect of iron-nickel cations on urea-assisted hydrothermal dechlorination of polyvinyl chloride: Appropriateness of using steel reactors for determining intrinsic degradation chemistry*. Pages 202-211.

Hydrothermal dechlorination of polyvinyl chloride (PVC) is primarily performed in stainless-steel reactors prone to chlorine-induced pitting corrosion, contaminating the reaction media with Fe2+, Ni2+, and Cr2+ possibly triggering shifts in the degradation chemistry. This study investigated the single and synergistic effects of Fe2+ and Ni2+ on urea-assisted hydrothermal dechlorination of PVC under mild conditions. Significant improvement in dechlorination degree was observed at 210 °C when 5 mmol/L Fe2+ or 10 mmol/L Ni2+ was added. Furthermore, positive interaction between the cations was confirmed when the simultaneous use of 1 mmol/L Fe2+ and 0.25 mmol/L Ni2+ achieved the same catalytic performance. The presence of these ions prevented adhesive contact of PVC particles, thus limiting the mass-transfer resistance and autocatalytic effect. The experimental design revealed that dechlorination and its improvement were temperature-dependent ($p < 0.0001$). Ni2+ and Fe2+ exerted quadratic and linear effects, respectively, on dechlorination. The highest catalytic activity occurred in the temperature range of 217.5–222.5 °C. The results show that total concentrations of as low as 1.08 mmol/L accelerated dechlorination, indicating the inappropriateness of using steel reactors for determining intrinsic PVC degradation chemistry. However, Fe–Ni composites have the potential to be used as catalysts.

- **Keywords:** Hydrothermal dechlorination; PVC; Response Surface Methodology; Catalytic effect; Synergy

Nicolas Abdel Karim Aramouni, Marina Steiner-Browne, Rabah Mouras. *Application of process analytical technology (PAT) in real-time monitoring of pharmaceutical cleaning process: Unveiling the cleaning mechanisms governing the cleaning-in-place (CIP)*. Pages 212-222.

We report for the first time the combination of inline process analytical technology and optical imaging to track and understand different cleaning mechanisms governing the cleaning process of Olanzapine. Clean-in-Place process parameters were studied through simultaneous inline process analytical technology and image analysis in a film flow apparatus. Methanol and water were compared as cleaning agents, and the effect of flow (0.5—1 L.min−1) and temperature (20–40 °C, and 60 °C for water) was investigated. The cleaning process was assessed in terms of cleaning time, volumetric efficiency, surface residue and governing phenomena. Raman spectroscopy was used to prove no degradation occurred during cleaning. Temperature increase improves the efficiency even when solubility is negligible. High variability was observed when detachment behaviour is dominant, and it is then advisable to prioritize dissolution in the final clean-in-place steps to improve repeatability. Results show that the cleaning process is governed by an interplay of dissolution and mechanical shear phenomena and is more efficient when solubility is significant. The combination of in-situ process analytical technology and optical imaging analysis during process development allows for the determination of the most efficient and repeatable conditions, which in turn significantly reduces solvent usage in pharmaceutical cleaning.

- **Keywords:** Pharmaceutical cleaning, Cleaning-in-Place (CIP); Cleaning validation, Olanzapine; Real-time monitoring, PAT; UV-vis

Andréia B. Santos, Alexandre Giacobbo, Marco Antônio S. Rodrigues, Andréa Moura Bernardes. *Integrated membrane process (UF/RO/EDI) for treating a petrochemical wastewater to obtain ultrapure water for industrial reuse*. Pages 223-231.

The scarcity and change in water quality reinforce the need to reuse effluents in water intensive industries as the petrochemical ones. In this article, the tertiary effluent from a Petrochemical Complex in Southern Brazil was used as feed water in a pilot unit with a capacity of 1 m^3 .h−1 to produce industrial water to be reused as clarified or demineralized water (ultra-pure water). For the treatment, an integrated system composed of ultrafiltration (UF), reverse osmosis (RO) and electrodeionization (EDI) was used. The parameters evaluated were aluminum, calcium, chloride, electrical conductivity (EC), color, chemical oxygen demand (COD), iron, magnesium, pH, total suspended solids (TSS), sulfate and turbidity. The UF/RO system operated with average permeate fluxes of 6.6 and 6.7 L.h−1.m−2, respectively. For the EDI, the operational parameters (flow rate, electric current and EC in the feed water) were optimized, considering the percentage of conductivity removal (%RC) as a response, by using response surface methodology (RSM) based on a central composite design (CCD). The best predicted values of flow rate, electric current and conductivity of the feed water were 6.6 L.min−1, 1.27 A, and 22.2 μS.cm−1, respectively. The %RC predicted in the software was 98.2%, similar to the mean value at the midpoint 97.1%. The EDI system was operated with the model conditions, and the product water reached the necessary quality to be reused as demineralized water in the Southern Petrochemical Complex in Brazil. Industrial reuse can reduce 20% raw water collection and 70% of the effluent volume disposed in the soil, thus reducing the water footprint, and increasing the sustainability of the petrochemical industry.

- **Keywords:** Petrochemical effluent; Reuse; Reverse osmosis; Electrodeionization; Ultra-pure water; Industrial sustainability

Aitao Zhou, Jiaying Hu, Kai Wang, Changang Du. *Analysis of fault orientation and gas migration characteristics in front of coal mining face: Implications for coal-gas outbursts*. Pages 232-245.

Coal in a natural geological mass is typically heterogeneous, potentially containing widely distributed faults that affect gas migration and are closely associated with the occurrence of coal-gas outbursts. In this study, the permeabilities of intact and heterogeneous coals during the mining process were described using a dual-porosity model and modified transversely isotropic permeability model, respectively. Numerical simulations based on these models revealed a high gas pressure gradient in front of the working face largely owing to the blocking effect of a low-permeability zone along the fault that led to the formation of a high-pressure gas zone; field measurements confirmed that the gas content in this zone was 2–3 times that in ordinary coal. When close to the fault, a considerable quantity of gas was observed within the working face, then the gas emission increased by 2.4 times once the low-permeability zone along the fault was obliterated. Finally, the proposed model was employed to explain how concurrent increases in shear stress and gas pressure affect the stability of a fault and promote coal-gas outbursts. The proposed model can be applied to conduct theoretical assessments informing measures to prevent gas-related dynamic disasters in coal mines.

- **Keywords:** Coal-gas outbursts; Coal permeability; Gas migration; Faults

Ibrahim M. Elsawy, Ahmed Hamoda, Swellam W. Sharshir, Ahmed Khalil. *Experimental study on optimized using activated agricultural wastes at hemispherical solar still for different types of water*. Pages 246-257.

The subsequent work aims to improve freshwater production and reduce the cost of generated water with little energy expenditure. Thermo-economic performance, hourly and daily production were evaluated by the experimental study on a hemispherical solar still in several configurations. The two floating agricultural waste materials utilized in the experiment were charcoal derived from guava tree wood (CHL) and carbonized corncobs (CCC). To enhance photothermal properties of the utilized primary materials, both have undergone physical and chemical activation by HCL or NaOH under specific conditions. In addition, the experiment was conducted using both seawater and lake water. Each modified distiller's performance was compared to that of a conventional unit in terms of thermal efficiency, exergy efficiency, daily output, and cost of freshwater in the climate of Kafrelsheikh, Egypt (31.09679°N, 30.94945°E) from 9:00 A.M. to 5:00 P.M. Therefore, this study aims to enhance the photothermal properties of charcoal and corn cobs by chemical and physical activation, which lead to enhance the efficiency of the hemispherical solar still by using this modified agricultural waste in its base compared to the traditional way. The daily productivity, thermal, and exergy efficiencies for H.CCC.LW were 4455 mL/m2,41.19%, and 3.85% showing improvement compared to a conventional hemispherical solar still by 41.2%, 40.72%, and 59.09%, respectively. At approximately 0.014 $/L (a savings of 26.70%), H.CCC.LW was shown to be the most cost-effective source of freshwater.

- **Keywords:** Thermal efficiency; Productivity; Hemispherical solar still; Activated agricultural waste; Water price; Charcoal; Corncobs

Fabin Zeng, Zhongan Jiang, Dengfeng Zheng, Mingli Si, Yapeng Wang. *Study on numerical simulation of leakage and diffusion law of parallel buried gas pipelines in tunnels*. Pages 258-277.

Parallel buried gas pipelines in tunnels are located in a confined space environment, where natural gas is vulnerable to accumulating to the minimum explosion limit concentration after a leakage accident. Therefore, to reduce the time for locating the leakage source after an accident and compensate for the loss of emergency response, an experimental model for scaling parallel gas transmission pipelines in tunnels was established and the dispersion characteristics and influencing factors of continuous leakage of natural gas within buried soil and in tunnel space were investigated numerically, and the correlation between the volume of the explosion range of natural gas within the tunnel space and each influencing factor was explored using gray correlation analysis. The research shows that the leakage dispersion process of parallel buried gas pipelines in tunnels includes seepage leakage in the soil region and diffusion transport in the tunnel air region. In the soil region, natural gas from the pipeline leak forms a circular shape and tends to percolate upward due to the combined effect of pressure and concentration gradients.In the tunnel air region, the spatial dispersion of natural gas concentration obeys a multivariate Gaussian distribution, and the temporal dimension is divided into three phases: the initial phase of leakage, the spreading phase and the stable phase of leakage. The diffusion speed of natural gas is positively correlated with the operating pressure of pipeline. The concentration peak value (ymax) at the leakage orifice position and the leakage aperture (dx) approximately meet the linear relationship: ymax= 7.62dx. The diffusion path of natural gas is greatly influenced by the orientation of the pipeline perforations, and the tunnel walls have a directional effect on the diffusion of natural gas. The main factors affecting the volume of the explosion range of natural gas within the tunnel space are parallel pipeline leakage pressure, pipeline leakage aperture, parallel pipeline leakage position, pipeline operating pressure, and pipeline leakage direction, with grey correlation coefficients of 0.76, 0.675, 0.662, 0.553, and 0.55. The proposed model was demonstrated be able to simulate and predict the diffusion of natural gas under the accidental leakage of buried gas pipelines in tunnels. And the results of this study can guide the installation of buried gas pipelines crossing mountain tunnels to prevent accidents.

- **Keywords:** Tunnel; Buried pipeline; Small hole leakage; Continuous diffusion; Experimental validation; Numerical simulation

Jialin Xu, Zhanguo Su, Junyan Meng, Yuzhong Yao, Mohammad Shahab Vafadaran, Ali Kiani Salavat. *A thermodynamic, exergoeconomic, and exergoenvironmental investigation and optimization on a novel geothermal trigeneration system to sustain a sport arena*. Pages 278-298.

In recent years, there has been a growing emphasis on sustainable energy provision for sport facilities, aiming to reduce carbon emissions, promote energy efficiency, and create a more sustainable sporting environment. The present investigation concurs with introducing a novel trigeneration system intended to generate power and provide heating and cooling load for sports facilities. The present system is offered to sustain the general energy requirement of an intended sport compound independently throughout the year. The single-flash Geothermal (SFG) system is included as a measure for attaining the required energy to initialize the system. After producing power and providing heat load, the remaining exergy associated with the SFG system is harvested and utilized to drive the double-effect absorption chiller (DEAC), Kalina cycle (KC), and the Organic Rankine cycle (ORC). A further study based on the first law of thermodynamics revealed that the SFG system, KC, and ORC allot thermal efficiency by 5.724 %, 9.31 %, and10.26 %, respectively. Furthermore, the second-law investigation determined that the SFG system,

KC, and ORC allocate exergetic efficiency by 18.08 %, 34.89 %, and 48.64 %, respectively. From an extended numerical perspective, the SFG system was deemed to result in a total output value of 66.55 kW worth of power and 615.8 kW worth of heating load. The DEAC performed with an 88.8 kW worth of cooling load provision and 1.199 as the coefficient of performance (COP). The KC and the ORC delivered 26.14 kW and 14.61 kW as in total outlet power, respectively. Integrally, the generalized system was found capable of producing 107.3 kW worth of net power output. The sum unit cost of the products (SUCP) was evaluated for the overall system, which equals 45.55$/GJ. A multi-objective Genetic algorithm optimization is carried out, aiming to achieve the optimal points and conditions of the system using the Pareto frontier method, where point C was chosen according to the TOPSIS criteria, deriving 46.0$/GJ and 40.09 % associated with SUCP and exergetic efficiency, respectively. Eventually, the exergoenvironmental parameters are derived and analyzed to study the environmental impacts.

- **Keywords:** Single-flash geothermal system; Organic Rankine cycle; Kalina cycle; Double-effect absorption chiller; Exergoenvironmental analysis; Pareto frontier

Yi Xu, Keqi Zhu, Xinyue Sun, Shumin Xu, Changhui Liu, Shenghua Xiong, Qichao Ran. *High mechanical flexible and recyclable organic-inorganic hybrid polyhexahydrotriazine aerogel for oil/water separation*. Pages 299-306.

Oily wastewater and light crude spills are great threats to the environment and human health, polymeric porous materials for oil/water separation is a very effective method to reduce environmental pollution and protect human health. Herein, we design recycle, super-hydrophobic, and mechanically flexible silicone-based polyhexahydrotriazine (Si-PHT) aerogel for efficient oil/water separation, hexanediamine-based polyhexahydrotriazine (HDA-PHT) is also designed for parallel comparison. The Si-PHT and HDA-PHT aerogels are obtained via the cross-linking reaction between diamine and formaldehyde, followed by the atmospheric drying without any additional post-processing. The as-prepared Si-PHT aerogel shows excellent hydrophobicity (water contact angle of 154.19°). Moreover, the adsorption capacity of Si-PHT aerogel for oil or organic solvent is 22.6–40.5 times of its own weight. More importantly, the Si-PHT aerogel could be compressed to 50% of its original size with outstanding high compress strain (554.3 kPa). The major raw material for synthesis of Si-PHT and HDA-PHT aerogels are readily recoverable and further recycle. This work provides a simple prepared and recyclable porous material for oil/water separation, and a rationally designed Si-PHT aerogel shows great potential for practical applications in the treatment of oily wastewater.

- **Keywords:** Recyclable; Superhydrophobicity; Mechanical flexible; Polyhexahydrotriazine aerogel; Oil/water separation

Tao Hai, Farhan A. Alenizi, Abdullah H. Alshahri, Bhupendra Singh Chauhan, Ahmed Sayed Mohammed Metwally, Hamad R. Almujibah. *Energy and environmental analyses of a sustainable multi-generation municipal solid waste-to-energy integrated system for hydrogen production*. Pages 307-321.

Municipal solid waste (MSW) management is a global challenge, and its efficient treatment is critical to reducing environmental pollution and greenhouse gas emissions. MSW-to-energy systems have emerged as a promising solution for sustainable waste management. Hydrogen production from MSW offers several benefits, including reducing reliance on fossil fuels, mitigating climate change, and promoting circular economy principles. The main aim of this study is to design and model an innovative integrated

energy system to convert an MSW stream to hydrogen in a multi-generation system. In this regard, a gas turbine cycle, a proton exchange membrane, and a supercritical carbon dioxide Brayton cycle are integrated and produce hydrogen, power, oxygen, heated air, and heated water. Energy and environmental analyses are implemented on the system and its performance is multi-objectively optimized using the Taguchi technique and the signal to noise analysis. The contributions of the input variables on the system performance are evaluated using the analysis of variance. Municipal solid waste of 1.75 kg/min, inlet turbine temperature of 850 °C, and pressure ratio of 10 are recognized as the optimum conditions. The system produces 472 kW of power, 57.7 g/min of hydrogen, 458 g/min of oxygen, 480 m3/min of heated air, and 12.2 L/min of heated water in the optimum state. The system presents the efficiency of 79.3% and emits 8.32 g/kW.min of carbon dioxide.

- **Keywords:** Environmental sustainability; Waste management; Waste-to-energy; Taguchi; Hydrogen production

Zhi Zhang, Shuai Fu, Mohammad Marefati. *A waste heat and liquefied natural gas cold energy recovery-based hybrid energy cycle: An effort to achieve superior thermodynamic and environmental performances*. Pages 322-339.

Cascading energy production cycles to make maximum utilization of waste heat can considerably enhance thermodynamic performance. In addition, the simultaneous recovery of waste heat of a power plant and liquefied natural gas (LNG) cold energy in the form of cascading power generation cycles can lead to superior thermodynamic and environmental results. In this article a comprehensive analysis of a solar-assisted hybrid energy cycle (HEC) for electricity and natural gas (NG) generation is presented. The developed HEC is comprised a tri-stage organic Rankine cycle (ORC) unit, a double-stage organic flash cycle (OFC) unit, and a solar unit based on parabolic trough collectors (PTCs). Exhaust gas, LNG, and solar energy are considered as main inputs. By employing the offered solar-assisted HEC, it is possible to take maximum advantage of the large temperature difference between the exhaust gas (CO2) and LNG. Besides, a percentage of the cycle's thermal duty is produced via the solar farm. A comprehensive analysis of thermodynamic, exergoenvironmental and exergoeconomic standpoints has been conducted. A tri-objective optimization algorithm and a sensitivity analysis considering all the above standpoints are also developed. According to the developed simulation, net output electricity, NG production rate, and exergy efficiency of the energy cycle were almost 8.63 MW, 22.62 kg/s, and 66.4%, respectively. Further, the values of product unit environmental impact and product unit cost were 0.262 mPts/kWh and 0.0923 USD/kWh, respectively. Moreover, elevating the compressor pressure ratio can greatly enhance the environmental impacts caused by the offered solar-assisted HEC. Also, raising the value of pressure ration of the compressor can greatly enhance the environmental impacts. Finally, the performance of the solar unit was done according to the solar radiation data of a certain city.

- **Keywords:** Exhaust gas; LNG cold energy; Solar thermal energy; Hybrid energy cycle; Exergoenvironmental; Exergoeconomic

Jianqi Chen, Rui Cai, Haitao Huang, Qi Wei, Bing Liu, Aosong Wei, Meng Zhang, Wenjie Lv, Hualin Wang. *Collaborative removal of fine catalysts particles and insoluble organics from methanol-to-olefins reaction wastewater using horizontal swirl regeneration micro-channel separation (HSRMS)*. Pages 340-354.

The methanol-to-olefins (MTO) process is regarded as a crucial approach for ensuring the sustainable growth of China's chemical industry. However, the fine catalyst particles and

insoluble organics in the water system poses a serious threat to the stability of the MTO process. A novel horizontal swirl regeneration micro-channel separation (HSRMS) method for purifying the MTO reaction wastewater was developed in this study. On-site experiments were conducted using a device with a capacity of 1 t/h to investigate the separation and regeneration effects under various parameters and to verify the feasibility of this method through a long-term observation. The results showed that this method could effectively remove the fine solids and insoluble organics in the reaction wastewater, and the device operated stably with fluctuations in both the quality and quantity of wastewater for 24 consecutive days. The suspended solids in the effluent was maintained below 5 mg/L, and the average removal efficiency for insoluble organics exceeded 75%. Furthermore, the excellent regeneration performance was achieved, with solid particles and oil in the media reduced to less than 0.2% after regeneration. This method could ensure long-term stable operation of the water system and outperform other commonly used reaction wastewater treatment methods in terms of investment, maintenance cost, freshwater supplementation, and energy consumption.

- **Keywords:** Hydrocyclone enhanced filtration; Depth filtration; Methanol-to-olefins; Oily wastewater; Micro waste catalyst

Mohammad Mahbubul Hassan. *Wash-durability, surface, and antibacterial properties of wool fabric treated with nature-derived thymol and totarol under subcritical CO2, aqueous, and ethanol media*. Pages 355-365.

Traditional aqueous-based antibacterial treatments used for wool fabrics are not sustainable as they produce toxic effluent and therefore it is necessary to develop a zero-effluent treatment. In this work, wool fabrics were treated with two plant-derived non-toxic antibacterial agents, thymol and totarol, under subcritical carbon dioxide (subc-CO2), and their antibacterial properties were measured. The wash-durability of the fabric treated with thymol under subc-CO2 was compared with wool fabrics treated with thymol in aqueous and ethanol media. The change in the physicochemical properties of the wool fabric treated with thymol under subc-CO2 at various concentrations was assessed by FTIR, contact angle measurement, and EDX spectroscopy. Thymol showed excellent antibacterial properties, but the wool fabric samples treated with totarol showed no antibacterial activity. The wool fabrics treated with thymol in the aqueous and ethanol media lost antibacterial activity after 5 times IWS 7A washes, but the fabric treated with thymol under subc-CO2 showed excellent antibacterial activity even after 20 times IWS 7A washes (equivalent to 80 domestic washes) indicating its high durability to wash. The thymol treatment slightly improved the hydrophobicity of the treated fabric's surface as the contact angle at 240 s improved to 119° for the fabric treated with 5% thymol from 106° for the untreated control fabric.

- **Keywords:** Sustainable zero-effluent treatment; Subcritical CO2; Thymol; Surface properties; Antibacterial properties

Shuaihua Guo, Zhiwei Wang, Gaofeng Chen, Mengju Zhang, Tanglei Sun, Qun Wang, Zhimin Du, Yan Chen, Mengge Wu, Zaifeng Li, Tingzhou Lei, Kiran R.G. Burra, Ashwani K. Gupta. *Co-pyrolysis characteristics of forestry and agricultural residues and waste plastics: Thermal decomposition and products distribution*. Pages 380-390.

Co-pyrolysis technology is an important realizable pathway for efficient resource utilization of different kinds of organic solid wastes. Thermogravimetric analysis (TGA), Fourier transform infrared spectrometer (FTIR), and pyrolyze coupled with gas chromatography/mass spectrometry (Py-GC/MS) were used to examine the thermal decomposition behavior, pyrolysis performance, and products distribution from different

kinds of solid wastes. Results are presented using agricultural and forestry residues (poplar biomass and rape straw), waste plastics (polyvinyl chloride and polystyrene) and their mixtures in 1:1 mass ratio. The TGA results showed a low comprehensive pyrolysis index (CPI) for the examined agricultural and forestry residues as compared to their mixtures with waste plastics that showed improved pyrolysis performance during their co-pyrolysis. The FTIR data of forestry and agricultural residues and waste plastics showed that they have a similar functional group (-CH3, -CH2, -CH and -C-). The possible occurrence of the products in the pyrolysis was further predicted by these functional groups. The results of Py-GC/MS analysis showed that the yield of aromatic hydrocarbons in co-pyrolysis of agricultural and forestry residues and waste plastics improved compared to solo pyrolysis of agricultural and forestry residues. The study provides efficient synergistic conversion of biomass and plastics for their treatment with favorable products distribution and yields.

- **Keywords:** Forestry residue; Agricultural residue; Waste plastics; Co-pyrolysis; Product characteristics

Luciana Melisa Del Gobbo, Juan Manuel Pérez Iglesias, César Américo Almeida, Liliana Beatriz Villegas, Verónica Leticia Colin. *Conversion of sugarcane vinasse into biomass of Aspergillus sp. V1 and its potential application as a fish feed ingredient*. Pages 391-399.

Vinasse generated by bioethanol industry is the acid liquid waste with high content of organic matter that causes undesirable impacts when it is poured into the ecosystem, indiscriminately. Therefore, the development of new technologies to improve the vinasse management is relevant worldwide. As a possible alternative, in this study, conversion of sugarcane vinasse into biomass of Aspergillus sp. V1 for use as a cheap fish feed ingredient was evaluated. Vinasse toxicity was also monitored, before and after biomass production, using growth parameters in Lactuca sativa as endpoints. Biomass of Aspergillus sp. V1 produced from vinasse supplemented with 2 g/L urea revealed a nutritional composition within recommended levels for fish diets, and an aflatoxins concentration of 12.9 μg/kg, which was within permissible levels for animal feeds. Fish feeding assays with 50 % and 100 % fungus biomass did not demonstrate any adverse effects for Poecilia reticulata, used as a model organism. Finally, inhibitory concentration (IC50) on L. sativa root elongation was 11.7 % for initially received vinasse and 23.8 % for vinasse resulting from biomass production. These findings demonstrate that it is feasible to minimize the transfer of distilleries pollution to the environment through biological conversion of vinasse into fungal biomass with nutritional value.

- **Keywords:** Vinasse management; Biological conversion; Fungus biomass composition; Fish feed ingredient; Body condition index; Assessment endpoints

Ahmet Bozgeyik, Lutfiye Altay, Arif Hepbasli. *Energetic, exergetic, exergoeconomic, environmental and sustainability analyses of a solar, geothermal and biomass based novel multi-generation system for production of power, hydrogen, heating, cooling and fresh water*. Pages 400-415.

The present study proposes and investigates a novel solar, geothermal and biomass based multi-generation system producing multiple outputs to generate power, hydrogen, heating, cooling, and fresh water. Parabolic trough solar collectors, a two stages Rankine cycle, two organic Rankine cycles, two absorption cooling systems, a gas turbine system, a once-through (OT) multi stage flash (MSF) desalination unit, a geothermal unit, a heat pump, an electrolyser and a thermal energy storage are used as sub-systems. The novelty of the system is to focus on novel sub-system design pattern for the proposed multi-generation system by using multiple energy inputs as there is a gap about those

studies in the literature. The overall system performance is evaluated from energetic, exergetic, exergo-economic, environmental (4E) and sustainability points of view by using the EES software package. The total installed power and hydrogen mass flow rates are 7.76 MW and 3.52 kg/h, respectively. The energy and exergy efficiency values of the overall system are found to be 65.55% and 27.09%. Fresh water flow rate is calculated to be 6.16 kg/s with 10 stages. The overall unit product cost is determined to be 21,79 $/GJ and the overall social ecologic factor is calculated to be 1.37.

- **Keywords:** Multi-generation; Exergo-economics; Renewable energy; Hydrogen; Desalination

Ruixue Xiao, Kefan Chao, Ju Liu, Li Wang, Muhua Chen, Xinbao Zhu, Bo Fu. Simulation of Rayleigh convection during dichloromethane absorption by water using lattice Boltzmann method. Pages 416-426.

Developing dichloromethane (DCM) waste gas purification and absorption technology is consistent with the demand of the circular economy and contributes to the goals of achieving carbon peaking and carbon neutrality. In addition, Rayleigh convection generated during the absorption of DCM by water is of great significance for understanding the interfacial mass transfer mechanism and enhancing the mass transfer efficiency. Thus, the absorption process of DCM discrete diffusion sources was simulated using the two-dimensional lattice Boltzmann method (LBM) with external forces to visualize the effect of Rayleigh convection evolution law on the mass transfer of the absorption process in this study. The concentration and velocity distribution with single or multiple diffusion sources were respectively simulated at 298.15 K and 1.00 atm. The results show that the convection structure of the simulated plume is similar to that of comparable studies, and the convective structure on both sides suppresses the development of the intermediate convective structure when convection occurs. At a constant gas-phase concentration (CB,g), the more the number of diffusion sources, the faster the convective structures integration, and the rapid integration of convective structures is associated with the sharp increasing instantaneous mass transfer flux. Meanwhile, increasing the gas phase concentration can effectively shorten the convection onset time (tc), increase the instantaneous mass transfer flux (Nins,t), and enhance the mass transfer efficiency by calculating the simulated transfer mass data. Furthermore, the critical onset time of Rayleigh convection first lengthens and then shortens with the number of diffusion sources (n) increasing. And the more the number of diffusion sources, the more significant the final cumulative (Nt) absorption amounts are. The simulation results can provide theoretical guidance for enhancing the mass transfer efficiency in the DCM absorption process.

- **Keywords:** Dichloromethane absorption; Lattice Boltzmann method; Rayleigh convection; Interfacial mass transfer

Wan Hanna Melini Wan Mohtar, Muhammad Amirul Mohd Razali, Muhammad Abid Mazlan, Arash Zulkarnain Ahmad Rozaini, Silambarasi A.P. Mooralitharan, Aidil Abdul Hamid, Muhamad Ramdzan Buyong. *Rapid detection of ESKAPE and enteric bacteria using tapered dielectrophoresis and their presence in urban water cycle*. Pages 427-435.

ESKAPE (Enterococcus faecium, Staphylococcus aureus, Klebsiella pneumoniae, Acinetobacter baumannii, Pseudomonas aeruginosa, and Enterobacter species) and enteric bacteria Shigella dysenteriae, Salmonella typhimurium and Escherichia Coli have been causing increasing nosocomial infections worldwide, contributing to high mortality and morbidity in surgical wards. This study attempts to investigate the feasibility of dieletrophoresis (DEP) electrode in detecting both ESKAPE and enteric bacteria in water

samples. The detection is based on the bacteria's response to the non-uniform electric field in micro tapered DEP electrode and microfluidic chamber. Responses of each bacterium were recorded by varying the frequency of sinusoidal 6 voltage (peak to peak) from 10 to 13,000 kHz. Utilising the unique electrokinetic responses of each bacterium, the performance of DEP application is assessed in detecting the ESKAPE and enteric bacteria from samples within the urban water cycle, i.e., wastewater, river, runoff, and treated water from an urbanised developed area. The positive (PDEP), negative (NDEP) and transitional, (denote as the crossover frequency fx0) responses for each bacterium were consistently determined, spanning between 52.3 and 12,000 kHz. DEP technique was successfully able to detect ESKAPE and enteric bacteria from water samples, where water from the river proved to be the most microbially contaminated in urban water cycle.

- **Keywords:** ESKAPE bacteria; Enteric bacteria; Dielectrophoresis; Crossover frequency

Yuntao Shi, Lei Zhao, Meng Zhou, Xiang Yin, Wei Guo, Chao Li. *A dynamic community gas risk-prediction method based on temporal knowledge graphs*. Pages 436-445.

This paper presents a community gas-safety risk-prediction method for solving the complex and continuous community gas-safety factors based on the temporal knowledge graphs. First, a community gas-safety risk-assessment index system is constructed based on the risk sources and factors influencing gas accidents. Entity and relationship features are extracted from the index system to construct a temporal knowledge graph of the community gas system. The community gas-safety risk-assessment index system is constructed based on the risk sources and risk-influencing factors of gas accidents. Furthermore, entity and relationship features are extracted in the index system to construct temporal knowledge graphs for a community gas system. Then, a gas-system risk-prediction method based on the temporal knowledge graphs is proposed, which predicts the risk level of the gas system in a certain period in the future. Finally, by applying the method in a specific community, the accuracy of the proposed prediction method is 74.87%, and the mean reciprocal rank is 87.44. The proposed gas-safety risk-prediction method based on a temporal knowledge graph network can assist managers in effectively managing community gas and has a positive auxiliary effect on sensing and controlling gas-safety situations.

- **Keywords:** Gas safety; Indicator system; Risk prediction; Temporal knowledge graphs

Alireza Jalali, Shaghayegh Tarabkhah, Amirreza Azad, Sepahdar Ansarinik, Mehdi Rezaei, Ahmad Parsaee, Erfan Baghani, Amin Khosravinejad, Ehsan Houshfar. *Maximal utilization of purge gas in methanol plants with improved primary furnace burners: A CFD study*. Pages 446-462.

The focus of this study is to achieve a better design of burners installed in petrochemical steam methane reformeing (SMR) furnaces. The initial design for the burners of the primary furnace in the Marjan petrochemical plant was problematic; hot spots occured on the side walls of the radiant chamber when the purge gas of the plant was added to the fuel stream. Three distinctive improvements have been recommended to alleviate this problem and provide higher combustion efficiency. These three suggestions include introducing pre-mixing of air and fuel streams, lowering the fuel nozzle velocity, and additional staggered nozzle holes to the base design to achieve more uniform flames. The non-premixed combustion computational fluid dynamics (CFD) simulations are conducted with ANSYS Fluent software on only one array of the burners, given the periodic

boundary conditions at the two sides of each array. The resulting temperature and velocity distributions are obtained to compare the designs. The results indicate that a more uniform temperature distribution will be achievable by adding the staggered nozzle holes, which provide a heat flux of 7604 W/m2 and reduce the radiant wall's average temperature by 0.598%. However, the combustion phenomenon occurs at its highest efficiency—99.998%—through the second design, where the fuel velocity is lowered at the nozzles. Although the first design with the pre-mixing of air and fuel performs more effectively in pushing flame towards the reformer tubes and reducing temperature variations along the radiant walls, the possibility of flash-back occurrence is high; so further safety actions must be taken into account. Eventually, the third design is chosen for implementation as economic analysis indicates that $10 million/year will be saved by lowering the amount of natural gas injected into the burners.

- **Keywords:** Steam Methane Reformer; Combustion; Burner; Methanol Plant; Flash-back

Yaoxuan Wang, Zhaoyang Zhang, Chuang Liu, Xiaolin Guo, Donghui Wei, Hongbing Du, Hong Wang, Shuai Wang, Yanxin Zhuang, Pengfei Xing. A clean process for preparing ferrosilicon alloy from coal gasification fine slag by carbothermal reduction processing. Pages 463-471.

The unreasonable treatment method of coal gasification fine slag (CGFS) in the industry has led to a serious waste of resources and environmental pollution, so it is of great significance to solve the problem. In this study, ferrosilicon alloy was successfully prepared from CGFS by carbothermal reduction processing, and the transformation of powdered CGFS to SiC-(Al2O3-CaO-SiO2) composite material was realized by the high-temperature vitrification process. The highest yield of ferrosilicon alloy was 35.23 % and the main compositions of the alloy were Si: 32.10 wt%, Fe: 60.52 wt%, Al: 1.93 wt%, Ca: 0.87 wt%, Ti: 2.56 wt% under the optimal smelting parameters: smelting temperature: 1800 °C; carbon content: 80 % of the theoretical value; holding time: 15 min. The final product slag was a mixed glass phase of SiC and Al2O3-CaO-SiO2, which can be used as raw material in ceramic materials preparation. Whether SiC is generated in large quantities has an important influence on the smelting process because the melted oxide will adhere to the SiC whiskers and limit the carbothermal reduction reaction. This work provides a theoretical foundation for the large-scale and high-value utilization of CGFS.

- **Keywords:** Coal gasification fine slag; Carbothermal reduction; Ferrosilicon alloy; Recycling

Mathiyazhagan Narayanan. *Origination, fate, accumulation, and impact, of microplastics in a marine ecosystem and bio/technological approach for remediation: a review*. Pages 472-485.

Plastic's widespread use in everyday life has resulted in massive amounts of plastic waste, posing a significant environmental burden. Microplastics have been widely dispersed throughout various ecosystems, and their microplastics pollution is already prevalent in marine ecosystems, contributing to an increase in awareness over the last few decades. More than 50% of all plastic pollution is disposed in landfills, with incineration accounting for almost one-fifth of all waste management. Nearly one-tenth of plastic debris is reused, with the remainder, approximately one-fifth of all improperly handled plastic waste, ending up in land and marine environments. A number of studies are being conducted to determine the source of microplastics along with their negative impact on marine organisms and, ultimately, human health. Hence, we compiled and scientifically discussed in this review the source, accumulation, and detrimental effects of microplastics on the marine ecosystem. Furthermore, the progress in bioremediation

options for microplastics remediation in marine aquatic ecosystems was thoroughly examined. It was discovered that growing scientific data reveals the existence of various forms of microplastics in food, and the aquatic ecosystem, as well as ultimately reaching humans. This review provides the collective information about the source and accumulation of microplastics as well as their impacts on aquatic organisms. Furthermore, in this review limitation in the microplastic detection and also research gaps in the remediation techniques were discussed. Furthermore, precise investigational research is required to support the negative effects of microplastics particles on human health. To address the microplastics pollution issues in marine environment, a few steps as well as attempts need to be taken. The knowledge gained from this review will serve as a foundation for future marine microplastics research and management techniques.

- **Keywords:** Microplastics; Marine aquatic system; Biodegradation; Microbial enzymes; Genetically modified organism

Bolin Sun, Ningjie Sun, Lu Wang, Yuan Li, Zhancheng Guo. *Efficient purification of scrap 1060 aluminum alloys contaminated with Fe and Si by super-gravity separation*. Pages 486-495.

1060 aluminum alloy has been used in high-volume commercial applications and correspondingly the mass of its downgraded recycling after contamination is huge, which is primarily due to the gradual accumulation of impurity elements such as Fe and Si. The separation of excess Fe is considered to be a key step towards the same-level recycling of aluminum alloy scrap with extremely economic and environmental benefits. A supergravity-induced technology was employed to purify the contaminating elements from molten aluminum scraps through Al2O3 CFF (Al2O3 ceramic foam filter). During the filtration process, the premature precipitation of Fe-rich phases and Si particles in the molten aluminum scraps were intercepted near the inner wall of Al2O3 CFF. Resultantly, the removal rate of Fe and Si reached 83.98 % and 49.67 %, respectively, at T = 690 ℃ and G= 30 via Al2O3 CFF of P = 80 ppi with H= 40 mm. A continuously supergravity-induced separation on industrial scale was further performed and the removal rate of Fe and Si were 83.5 % and 48.3 %, respectively.

- **Keywords:** 1060 aluminum alloy scrap; Purification; Super-gravity; Filter mediums; Al2O3 CFF

Chengyue Yang, Ziye Li, Zhuang Hu, Yu Sun, Feng Chen, Tuanyu Guo, Jianshe Hu. *Multifunctional 3D PAN-C3N4 @COFs for efficiently dynamic and static adsorption of mercury and its chemometric detection*. Pages 496-506.

In this study, we prepared a 3D aerogel, PAN-C3N4, using polyacrylonitrile (PAN) and C3N4 as raw materials through a hydrothermal method. Subsequently, a layer of COFs (FT) was grown on its surface. We modeled its structure and compared it with experimental PXRD patterns to obtain the possible final crystal structure. Afterward, through functionalization with butyne, we prepared a 3D aerogel composite, PAN-C3N4@FT@Butyne, which can be applied to the adsorption of both mercury(II) and elemental mercury vapor. In a short span of time (25 min), the maximum adsorption capacities of mercury(II) and elemental mercury vapor were found to be as high as 830.1 mg/g and 463 mg/g, respectively. Importantly, in the fixed-bed column study, the influence of flow rate and initial concentration of mercury(II) was evaluated through breakthrough curves, yielding an adsorption capacity of 25.48 mg/g. Meanwhile, the application of the fixed bed column for industrial wastewater treatment displayed exceptional adsorptive capabilities, reduced the concentration of mercury (II) from 10.0 mg/L to less than 1.76 μg/L, significantly below the permissible limit for drinking water (2 μg/L). In addition, PAN-C3N4@FT@Butyne can be utilized as a chemodosimeter

to detect mercury(II) in solution within a mere 5 s, with a detection limit of 0.1 ppb. Furthermore, COFs (BT) were cultivated within the PAN-C3N4 matrix as a control group, thereby demonstrating the widespread applicability of this strategy.

- **Keywords:** Mercury; Adsorption; Chemodosimeter; COFs; Fixed-bed column

Amin Alizadeh, Shakiba Asghar, Mostafa Roudgar-Amoli, Zahra Shariatinia. *Water remediation using activated montmorillonite/metal-organic framework nanocomposites: Response surface methodology, kinetic, and thermodynamic studies*. Pages 507-529.

The presence of dye pollutants in effluents is a significant concern due to their adverse effects on many life forms. For the purpose of removing Methylene Blue (MB) from an aqueous solution through the adsorption process, the H-MMT/MOF-5 and H-MMT/MOF-199 composites (MMT = montmorillonite, MOF = metal-organic framework) were produced. Composites made with diverse H-MMT: MOF (w/w %) ratios were used for the MB dye removal to study their adsorption characteristics over a 0–30 min time range. The 60 % H-MMT/40 % MOF-5 % and 70 % H-MMT/30 % MOF-199 composites showed the greatest amounts of MB removal. The effects of contact time, adsorbent dose, pH, and initial MB concentration on the removal of MB were studied using the central composite design (CCD) method. The process was studied using Response Surface Methodology (RSM) technique to optimize the adsorption process, and the optimum conditions were identified. For 60 % H-MMT/40 % MOF-5 % and 70 % H-MMT/30 % MOF-199, optimum MB removals of 97.52 % and 98.73 % with maximum adsorption capacities (qmax) of 192.3 and 238.09 mg g−1 were obtained. The experimental data of MB adsorption on H-MMT/MOF-5 and H-MMT/MOF-199 composites followed the Langmuir isotherm and pseudo-second-order kinetic model. Thermodynamic study demonstrated exothermic and spontaneous characters of the adsorption process. Also, MB adsorption by H-MMT/MOF-5 and H-MMT/MOF-199 composites was happened by electrostatic attraction, π-π interactions, and hydrogen bonding. The H-MMT/MOF-5 and H-MMT/MOF-199 composites based on a clay mineral H-MMT with greater specific surface area and reactive -OH groups are effective materials for developing low-cost and ecologically friendly adsorbents. According to the leaching test, H-MMT/MOF-5 and H-MMT/MOF-199 adsorbents presented good stability at pH values above 5. Therefore, the synthesized H-MMT/MOF-5 and H-MMT/MOF-199 composites could be effectively used to remove MB from water.

- **Keywords:** H-MMT/MOF-5 composites; H-MMT/MOF-199 composites; Methylene blue; Water treatment; Response surface methodology

Zhiqing Zhang, Rui Dong, Dongli Tan, Bin Zhang. *Multi-objective optimization of performance characteristic of diesel particulate filter for a diesel engine by RSM-MOPSO during soot loading*. Pages 530-545.

Diesel particulate filter (DPF) is one of the effective technologies for controlling vehicle particulate matter (PM) emissions. In this research, a hybrid multi-objective optimization approach of FGRA-RSM-MOPSO was developed for DPF, with optimization objectives including maximum initial filtration efficiency and minimum pressure drop. Decision variables include diameter, length, wall thickness, porosity, and pore diameter. Firstly, a computational fluid dynamics (CFD) model for DPF was established, and sensitivity analysis of DPF structural parameters was conducted through fuzzy grey relational analysis (FGRA) to screen out key factors affecting DPF trap performance. Then, response surface methodology (RSM) was used to establish the mathematical relationship between key structural parameters, initial filtration efficiency, and pressure drop. Finally, multi-objective particle swarm optimization (MOPSO) is used to optimize the target and select the optimal solution from the Pareto front. Compared with the

original DPF, the optimized DPF under standard operating conditions increased the initial filtration efficiency by 46.85% and reduced the pressure drop by 34.88%. The optimization effect is more pronounced under high load conditions.

- **Keywords:** Diesel particulate filter; Multi-objective optimization; Pressure drop; Filtration efficiency

Boxun Zhou, Zhaoji Zhang. *Desalination performance of shale gas produced water by flow-electrode capacitive deionisation process*. Pages 546-555.

The cost-effective desalination of shale-gas produced water (PW) has long been an industrial research hotspot. Flow-electrode capacitive deionisation (FCDI), a recently developed electrochemical desalination technology, may be a novel option for PW disposal because of its attractive advantages. However, reports on the desalination test of actual high-salinity industrial wastewater by FCDI are lacking. In this study, a laboratory-scale FCDI device with an online monitoring system was used to desalinate shale-gas PW. FCDI achieved relatively stable desalination efficiency for pretreated PW with a salinity of 2.65 % and reached an energy-normalised salt removal of 0.479 mg/J. The flow electrode chemically activated by KOH increased the FCDI average desalination rate by 98.5 % for the pretreated saline PW. Electrochemical impedance spectroscopy analysis revealed that the majority of fouling accumulated on the anion-exchange membrane (AEM) side. Residual pollutants were adsorbed by the flow electrode in the AEM chamber, which destroyed the optimal ion-transport path and electric double-layer structure. Results showed that FCDI was more suitable for PW's reverse-osmosis (RO) permeate desalination to form an RO–FCDI hybrid. This study provided a practical experimental case on the electrochemical desalination of saline PW by FCDI.

- **Keywords:** Flow-electrode capacitive deionisation (FCDI); Shale gas produced water; Desalination; Electrochemical impedance spectroscopy

Linlong Hu, Gongxing Yan, Bhupendra Singh Chauhan, Ibrahim Elbadawy, Mohamed Abouelela, Mohammad Marefati, Bashir Salah. *Development and evaluation of an electro-Fenton-based integrated hydrogen production and wastewater treatment plant coupled with the solar and electrodialysis units*. Pages 568-580.

The development of plants for the simultaneous production of green energy and clean water, in addition to improving the energy system performance, can facilitate the achievement of sustainable development. Meanwhile, hydrogen is one of the promising fuels that can overcome the intermittent penalties of renewable energy sources. In addition, due to environmental restrictions, the industry is forced to effectively treat wastewater for reuse. This article describes the evaluation of an economic model and optimization of an integrated hydrogen production and wastewater treatment plant based on an electro-Fenton process (EFP)-based photoelectrochemical stack (PES), a solar unit, and an electrodialysis unit. The wastewater supplied to the plant is the effluent of a textile factory. In addition, a concentrating photovoltaic thermal collector (CPVT) has been used as a solar unit in the plant. In the offered plant, the electrodialysis unit is able to produce the required alkaline and acid of the PES unit as well as desalinated water. The developed economic model is based on estimating the cost of hydrogen production per kilogram of hydrogen output (i.e., Levelized Cost of Hydrogen, LCOH) on a large scale plant (1072 kg H2/day). In this regard, approximately 230 m3/day of wastewater from the textile factory is treated. Relying on the proposed process can minimize the external chemical requirements of the hydrogen production and wastewater treatment plant. The value of LCOH for the planned plant was estimated to be 5.16 USD/kgH2. However, under the developed optimization, the LCOH value can be declined by almost

7.6%. According to calculations, the profitability of the wastewater treatment process can be approximately 0.082 M USD per year. It was also found that, the value of LCOH exhibits the most sensitivity to variations in operating capacity factor and the least sensitivity to variations in utilities consumption rate. A sensitivity analysis is also developed to identify effective solutions in evaluating the economic performance of the planned plant.

- **Keywords:** Hydrogen production; Wastewater treatment; Desalinated water; Solar energy; Economic model; Optimization

Zhangyu Cuan, Youming Chen, M. Saravana Kumar. *Design, multi-aspect analyses, and multi-objective optimization of a novel trigeneration system based on geothermal and municipal solid waste energies*. Pages 581-597.

The study of multi-source energy systems, due to higher performance and producing various products, is an interesting subject. The current study designs a multi-source system including a gas turbine cycle with CH4 and municipal solid waste digester, a geothermal system with an organic Rankine, organic flash, and a double-effect absorption refrigeration subsystem to produce power, cooling, and heating loads simultaneously. The thermodynamic and economic analyses are utilized to estimate the system's performance and multi-objective optimization has been applied to define the optimum state of the system concerning two scenarios. The results indicate that the system provides 423.4 kW net power, 384.7 kW heating load, and 106.3 kW cooling load with 39.28% exergetic efficiency and 6.67 years payback period. These values are improved to 664.9 kW net power, 446.5 heating load, 42.01% exergetic efficiency, and 6.05 years payback period at the best optimum scenario. The sensitivity analysis reveals that the air compressor's pressure ratio mainly impacts the net power, heating load production, and net present value. The cooling load production and exergetic efficiency are mainly affected by the air preheater effectiveness variation.

- **Keywords:** Municipal solid waste; Geothermal system; Double-effect absorption refrigeration cycle; Multi-source system; Multi-objective optimization

Mo Kuang, Da Kuang, Bashir Salah, Khieu Van Khai. *Examining the feasibility of a bi-evaporator cooling/electricity cycle: A comprehensive analysis of thermodynamic, economic, and environmental aspects, and bi-objective optimization*. Pages 598-616.

Although geothermal energy is generally considered benign, it still has its share of problems, including the emission of greenhouse gases that harm the environment. To make informed decisions about geothermal systems, it is imperative to study their environmental impacts. This study uses six approaches to propose and analyze an innovative geothermal-driven bi-evaporator cooling/electricity plan. The proposed efficient design is made of a single-flash cycle and the integration of a modified vapor compression cycle and ejector cooling system assisted by a thermoelectric power generator device. Exergoenvironmental and extended-environmental assessments are performed to examine the environmental impacts of the current devised scheme, including calculating CO2 emissions rate and sustainability index. The suggested plan's performance in the basic design mode using 14 various working fluids showed that R143m had the highest exergetic efficiency, lowest exergoenvironmental index, and lowest cost of production at 35.9%, 0.6002, and 24.67$/GJ, respectively. This working fluid was used for parametric study and bi-objective optimization, which revealed that the vapor generator destroys 157.7 kW of exergy at the optimal point. Additionally, the vapor turbine is the most expensive component at 14.44$/h. Pareto frontier also indicates that the final chosen optimal mode (scenario C) has 27.02% energetic

efficiency and 21.33$/GJ production cost, which are higher than the base scenario by 12.55% and 15.66%, respectively. In addition, the optimal scenario reduces the payback period to 8.64 years from 15.68 years in the base scenario.

- **Keywords:** Bi-evaporator cooling/electricity cycle; Exergoeconomic; Exergoenvironmental; Payback period; Pareto frontier

Kaixuan Wang, Xin Qin, Peike Cao, Shuo Chen, Hongtao Yu, Xie Quan. *High-efficiency refractory organic pollutants removal boosted by combining heterogeneous electro-Fenton with electrochemical anodic oxidation over a broad pH range*. Pages 635-642.

Electrochemical anodic oxidation (AO) is a green and efficient treatment process for refractory pollutants degradation. The cathode in AO process generally serves as the counter electrode, and does not contribute significantly for pollutants removal. The heterogeneous electro-Fenton (EF) process uses the bifunctional catalytic material as cathode to produce H2O2 via 2e- oxygen reduction reaction and activate H2O2 decomposition to generate •OH for degrading pollutants. Herein, we investigated an integrated electrocatalytic process between heterogeneous EF and AO (EF+AO) to enhance refractory pollutants removal over a broad pH range without the production of iron-containing sludge. Total organic carbon removal of phenol by EF+AO was 98.2 % in 180 min under pH ~5.9 and the applied current density of 1.0 mA cm−2, obviously higher than that of only EF (48.8 %) or AO (56.9 %). Significantly, EF+AO process can efficiently treat the actual coking wastewater that the chemical oxygen demand (COD) value gradually decreased from 312.3 mg L−1 to 47.8 mg L−1 with the low specific energy consumption of 14.0 – 25.7 kWh·(kg COD)−1. This process delivered excellent long-term durability in flow mode, retaining efficient degradation performance for phenol during 100 h of consecutive runs. Our results provide new insights into developing an energy-efficient electrocatalytic process for pollutants removal.

- **Keywords:** Oxygen-doped carbon nanotubes; Hydrogen peroxide; Hydroxyl radical; Ti/SnO2-Sb; Direct oxidation

Arash Esmaeili, Taeksang Yoon, Tesfalem Aregawi Atsbha, Chul-Jin Lee. *Rate-based modeling and energy optimization of acid gas removal from natural gas stream using various amine solutions*. Pages 643-663.

Reduction in energy consumption of industrial plants is always an essential need due to high cost, CO2 emissions and global warming caused by energy supply from fossil fuels for boilers and electricity consumers. Iran has been struggling to compensate the lack of gas supply for domestic and industrial demands in winter within the past decade despite of having large natural gas resources. One of the most economical methods to decrease energy requirements in hydrocarbon plants is process improvement and revamping by changing existing solvents. There are already 44 identical acid gas removal units under operation in the South Pars Gas Complex (located in Iran) with the same feed composition. The gas-sweetening unit in the Phase 12, operating with the solution of 45.5 wt% methyldiethanolamine (MDEA), was modeled by Aspen Plus for acid gas removal (CO2 and H2S) as a rate-based model with the application of electrolyte non–random two–liquid (E-NRTL) activity model and Peng–Robinson equation of state in addition to the actual characteristics of the absorber and regenerator, and the operational conditions of the gas and liquid streams. After validation of the model by the real data from the plant, the incumbent amine solution was replaced with five proposed amine solutions – one single and four blended amine mixtures – in the same mass concentration to select the most efficient alternative from the aspects of outlet acid gas concentration, H2S content in the treated flash gas, required total power, reboiler power supply, and regeneration heat duty. The simulation results revealed that H2S was sharply

absorbed on the top of the column, while CO2 was smoothly removed from the gas phase to the MDEA and blended solutions along the absorber and it occurred at the bottom of the column for the DEA solution. The blended amine solution of 1.5 wt% sulfolane + 44 wt% MDEA (Sulfinol-M) has shown to be the most appropriate option instead of the solution of MDEA compared to other suggested absorbents, with several advantages such as higher selectivity of H2S over CO2, low temperature bulge, highest H2S loading, and outlet sweet gas flow rate while required total power, reboiler power supply, and regeneration heat duty were reduced by 21.19%, 21.26%, and 23.54% respectively. The operational conditions of the unit with the application of the Sulfinol-M solution were optimized to achieve three specifications (constraints) and the minimum required total power (objective function) through a sensitivity analysis and optimization using a genetic algorithm to assure the reliability of values for three independent parameters, namely, amine solution temperature, amine solution flow rate, and gas temperature. The optimum limits and values of these parameters were 47–50 °C, 220 – 240 ton/h, and 34 °C respectively.

- **Keywords:** Acid gas absorption; Aspen Plus; MATLAB; Piperazine; Regeneration heat duty; Sulfinol-M

A.G. Olabi, Mohammad Ali Abdelkareem, Mohamed S. Mahmoud, Khaled Elsaid, Khaled Obaideen, Hegazy Rezk, Tabbi Wilberforce, Tasnim Eisa, Kyu-Jung Chae, Enas Taha Sayed. *Green hydrogen: Pathways, roadmap, and role in achieving sustainable development goals*. Pages 664-687.

The United Nations Sustainable Development Goals (UN-SDGs) provide a unique opportunity to achieve sustainable development and reduce climate change impact. Decarbonizing the energy system is a key approach to achieving the energy balance. Recently, green hydrogen has become the most promising energy source for decarbonizing energy systems. Therefore, determining the different production methods of green hydrogen, their economics, and their environmental impacts is essential to all stakeholders. Additionally, understanding the role of green hydrogen in achieving the different SDGs is vital for policymakers and decision-makers. Thus, this study reviewed the common hydrogen production methods. The prospect of achieving the SDGs has also been investigated, and the most relevant keywords were presented. Finally, a list of indicators (guidelines) to increase the green hydrogen contribution to the SDGs was provided. The provided indicators will assist the stakeholder in increasing the integration of green hydrogen into the SDGs and reduce the trade-off.

- **Keywords:** Green hydrogen; Production methods; Sustainable Development Goals; Indicators

Shi-zhou Li, Yang-fan Cheng, Rui Wang, Meng Li, Run Li, Hong-hao Ma. *Suppression effects and mechanisms of three typical solid suppressants on titanium hydride dust explosions*. Pages 688-698.

The suppression effects of melamine polyphosphate, titanium dioxide and melamine cyanurate powders on titanium hydride dust explosions were studied using a 1.2 L standard Hartmann tube system, a 20-L spherical vessel testing system, a simultaneous thermal analyzer and a field emission scanning electron microscope. The experimental results showed that the three solid suppressants could effectively decrease the explosion parameters such as flame luminescence intensity, flame propagation velocity and maximum explosion pressure, et al. Because of the different suppression characteristics of the suppressants, their suppression effects on the particles combustion temperatures were significantly different. To completely suppress the dust explosion of titanium hydride, the inerting ratio of the melamine polyphosphate powders was the smallest when compared with those of the titanium dioxide and melamine cyanurate powders. In

addition, the field emission scanning electron microscope was used to analyze the residues of a dust explosion. The testing results showed that the thermal decomposition residues of melamine polyphosphate powders were coating on the surface of the unburned titanium hydride particles to make them lose reactivity, that was why the suppression effect of melamine polyphosphate powders was the most effective when compared with titanium dioxide and melamine cyanurate powders.

- **Keywords:** Titanium hydride dust; Dust explosion; Solid suppressant; Suppression effect; Suppression mechanism

Ruiyan Ni, Jing Meng, Meiru Cheng, Qinfei Ke, Yaru Zhao, Xian Li, Yi Zhao. *Recent advances of proteins extracted from agricultural and livestock wastes in biodegradable textile sizing applications*. Pages 699-710.

Proteins from agricultural and livestock wastes are rapidly emerging as potential alternatives for non-biodegradable PVA sizes due to their excellent film-forming ability, amphiphilic, biodegradable, low cost and low carbon footprint. However, brittleness of protein-based films that failed to be directly used as textile sizing to protect yarns during high-speed weaving limits their practical applications. Different methodologies to modify protein-based materials to impart excellent properties are highly desired to be better used in textile sizing. Therefore, in this review, recent advances in the various modification methods of proteins and its applications in textile sizing have been focused. The categories, structure, methodology and characterization of modified-protein are fully covered. This review provides an overview of recent research advances on different protein-based textile sizing agents and promotes the development of a new generation of multifunctional bio-based materials from biological renewable resources and sustainability of the textile industry.

- **Keywords:** Proteins; Slurry; Textile sizing; Biodegradable; Modification

Kexin Yin, Tianxiong Liu, Yasen Dai, Guoxuan Li, Jianhui Zhong, Yuyang Jiao, Peizhe Cui, Zhaoyou Zhu, Yinglong Wang, Zhigang Lei. *A new correlation model of entrainer properties and process economics for ternary azeotrope separation by extractive distillation*. Pages 711-724.

A correlation model was explored and established for the first time, linking the properties of entrainers to the process economics of extractive distillation separation for ternary azeotropes. Firstly, the extraction process of ternary azeotrope (methyl tert-butyl ether/ethanol (EtOH)/water) with common entrainers was optimized using a multi-objective optimization method based on a genetic algorithm. The optimal process parameters were obtained, and dimethyl sulfolone emerged as the best entrainer for the system. An economic correlation model was developed using machine learning to link the properties of entrainers and total annual cost (TAC). The model exhibited a determination coefficient of 0.993 and a single percentage error of less than 2% for each data set, indicating a significant fitting degree and prediction accuracy. The feasibility of selecting the optimal entrainer and calculating the economic benefit of the model was verified through another ternary azeotrope system (i.e., tetrahydrofuran/EtOH/water). The model provides valuable insights into energy savings and entrainer screening in extractive distillation. Additionally, the influence of the heat integration process with different entrainers on the economic benefit was analyzed, and the optimum entrainer changed to glycerol after the heat integration process. This finding suggests that determining the optimum entrainer should consider the possible heat integration process design. Finally, the relationship between the intermolecular interaction mechanism and separation effect was revealed through quantum chemical calculations.

- **Keywords:** Extractive distillation; Multi-objective optimization; Molecular dynamics simulation; Separation mechanism; Machine learning

Xiaoxia Ye, Yi Lin, Wang Lin, Huiting Lin, Yuancai Lv, Chunxiang Lin, Yifan Liu, Jie Chen. *Biomass-derived foams with three-dimensional hierarchical structure for efficient p-arsanilic acid removal*. Pages 725-733.

As an emerging micro-pollutant, p-arsanilic acid (p-ASA) exist widely in the environment, and it can form highly toxic arsenate and arsenite during the migration and transformation process, which greatly increases the risk of arsenic pollution in the ecosystem. Additionally, three-dimensional (3D) porous block materials have the advantage of stronger adsorption performance, faster adsorption rate and easy recovery, showing broad application prospects in water pollution control. Hence, the aminozed collagen fibers foam (ACFF) with 3D porous block structure was synthesized. The maximum adsorption capacity of ACFF for p-ASA was 476.19 mg·g−1 due to the rich honeycomb porous structure and the synergistic effect of electrostatic attraction, hydrogen bonding effect and amphiphilicity. Moreover, ACFF is not only easy to recycle, but also has good elastic recovery and regeneration performance. The pore size of ACFF was concentrated in the range of 25–5000 nm, and the porosity was 71.66%. ACFF may be an adsorbent with great potential for the removal of organoarsenic contaminants in water.

- **Keywords:** p-arsanilic acid; Amphiphilicity; Three-dimensional (3D) porous block material; Continuous separation

Tao Chen, Dan Zhou, Zhaijun Lu, Shi Meng. *Experimental study on prediction models of diffusion flame geometry in moving fires*. Pages 741-751.

Flame geometry is a fundamental problem in assessing the thermal hazard during the transport process of hazardous chemicals, while the existing literature mainly focuses on stationary fires, with little understanding of flame behavior in moving fires. The objective of this study is to address the air entrainment mechanism of moving fires and derive the characterization models of relevant flame parameters. Dimensional analysis was used to determine the main factors influencing flame geometry in moving fires. A 1:10 scale burning car was then designed, and a series of moving model experiments were conducted to investigate the flame geometry. The results show that the flame height decreases monotonically with the increasing moving velocity, while the flame tilt angle gradually increases to a constant value. The variation of the flame width and the flame length includes three regimes: the decreasing regime, the transition regime, and the increasing regime. The evolution mechanism of the flame geometry can be attributed to the competition between the buoyancy and the inertia forces, which forms the bilateral, unilateral, and enhanced unilateral entrainment modes. Dimensionless correlations are provided to describe the flame geometries. Comparison between previous wind-blown flame models and the experimental data suggests that considerable error exists when studying moving fires by using wind tunnel experiments, despite their applicability to relevant aerodynamics studies.

- **Keywords:** Moving fire; Dimensional analysis; Moving model experiment; Flame geometry; Modelling

Lanbin Wang, Yangming Xu, Yanping Ma, Yu Chen, Anju Yang, Guixiang Gan, Yaguang Du, Yan Sun. *Detoxification and resource utilization of soda ash chromite ore processing residue by copper slag*. Pages 752-764.

Chromite ore processing residue (COPR) and copper slag (CS) are industrial waste slags that cause environmental pollution and require effective treatment. This study proposes a new strategy for the co-treatment and resource utilization of COPR and CS. Under the optimal conditions (liquid-solid ratio of 9.99; H2SO4 concentration of 0.85 M; the CS/COPR mass ratio of 9.98%; temperature of 88.20 ℃; and duration of 60 min), the reduction efficiency of Cr(VI) reached 99.48%, and the total Cr leaching concentration of residue reached 1.35 mg/L, which was below the USEPA regulatory limit of 5 mg/L. In addition, the detoxicated slag containing 61.44 wt% Fe2O3 can be used as a raw material in the steel industry. Through kinetic, characterization, and DFT analyses, the effective remediation of Cr(VI) in COPR by CS is a combination of adsorption and reduction. The unreacted shrinkage nuclear reaction model under the control of the surface chemical reaction is the most suitable model to describe the process, and when the apparent activation energy is 63.90 kJ/mol, the apparent rate equation is:1-(1-x)1/3= 1·371×107[CS/COPR]2·35004 [H2SO4]2·3945 [L/S]1·95338 exp(−63·90/RT)This is an important study for waste-waste co-treatment and resource utilization of industrial waste.

- **Keywords:** Chromite ore processing residue; Copper slag; Detoxification; Resource utilization

Zijun Li, Kai-Qi Zhong, Yu Xu, Yin Chen, Xiaowei Zhai, Yang Xiao, Gang Li. *Intermittent injection of carbon dioxide to control the risk of coal spontaneous combustion and methane explosion: A case study in U-type ventilation*. Pages 795-806.

The compound risk of coal spontaneous combustion (CSC) and methane (CH4) explosion poses a serious threat to mining safety. Green resource utilization of carbon dioxide (CO2) can help achieve carbon neutrality. Therefore, CO2 is seen as a means to prevent compound risk of CSC and CH4 explosion. To address the situation at the 4209 working face, a multi-physical field coupling model was established to simulate the CSC and CH4 explosion in the gob of a U-type ventilation system. The accuracy of the model was verified against measured data from the gob. Following the injection of CO2 into the gob, the volume of the compound risk area was significantly reduced. The effects of intermittent CO2 injection were compared to those of continuous injection, and it was determined that intermittent injection was the preferred method, taking injection cost into account. Three injection frequencies were tested, with F= 1/2 d showing the optimal effect. When the injection frequency was set to F= 1/2 d, and three CO2 injection flow rates were tested, it was demonstrated that a flow rate of 141.3 m3/h provided the most effective risk reduction while meeting the required CO2 concentration in the working face.

- **Keywords:** Compound risk; Carbon dioxide; Multi-physical field coupling model; Intermittent injection; Injection cost

Shuo Zhang, Yanqiu Pan, Wei Wang, Runze Lin, Xuewu Liu. *Carboxylated cellulose-based aerogel with cellular pores prepared by stir freezing for cationic dye adsorption*. Pages 807-817.

A TEMPO-oxidized cellulose (TOC)/nanofiber cellulose (NFC) biomass aerogel was prepared through freeze-drying (FD) for cationic dye adsorption. The stir freezing method was utilized to build cellular pores so as to improve the mechanical property of aerogel.

The dielectric-assisted microwave (MW) heating was adopted to increase the FD rate. The results showed that the proposed method could simultaneously intensify the mass and heat transfer of FD, reducing more than 36% of drying time. The TOC/NFC aerogel exhibited a high mechanical property with 91.36 kPa of compressive stress at 80% strain. The maximum adsorption capabilities of aerogel prepared by stir freezing for methylene blue (MB) and malachite green (MG) dyes were 248.27 and 227.30 mg·g−1, respectively. The prepared aerogel showed high selective adsorption of cationic dyes in binary dye solutions. Moreover, the prepared aerogel exhibited a satisfactory recycling performance in 20 cycles of adsorption/desorption experiments. This work provides a new freezing and FD strategy to prepare TOC/NFC aerogels with promising applications in industrial printing and dyeing wastewater treatment.

- **Keywords:** Biomass aerogel; Stir freezing; Microwave heating; Drying time; Dye adsorption

Mengfan Chen, Yulian Han, Congting Sun, Nanxun Jin, Youtao Song. *Rapid degradation of organic pollutants by enhanced persulfate activation using CeO2-MnFe2O4 nanostructures: A polymetallic synergistic effect*. Pages 818-830.

Persulfate-based advanced oxidation processes (AOPs) have attracted considerable attention in the treatment of organic wastewater with high performance and long lifetime. The construction of efficient, environmentally-friend, and stable nanocatalysts has been recognized as a promising approach to activate persulfate. Herein, magnetic CeO2-MnFe2O4 nanomaterials fabricated via a simple sol-gel method were used for the first time to enhanced activate persulfate (PS) for the removal of the organic pollutant enrofloxacin (ENR). It was demonstrated that 97.2% of ENR (10 mg L−1) was efficiently degraded. 63.3% of TOC decreased within 35 min under a neutral solution (pH 6.81) in the PS+CeO2-0.2MnFe2O4 system using a catalyst dosage of 0.25 g L−1 and 0.18 mM PS. The magnetic CeO2-MnFe2O4 nanostructures maintained excellent recovery as well as recyclability ENR removal efficiency was 90% after recycling five times. EPR and quenching tests indicated that sulfate radicals (SO4•−) and hydroxyl radicals (•OH) significantly contributed to ENR removal. XPS analysis showed that the synergistic redox cycles of Ce3+/Ce4+, Mn2+/Mn3+, and Fe2+/Fe3+ are essential to activate PS for ENR degradation. DFT calculations also revealed that PS molecules preferred to adsorb to and dissociate on CeO2-MnFe2O4 surfaces rather than just CeO2 and MnFe2O4 surfaces. CeO2 plays a dual role in the charge transfer from CeO2-MnFe2O4 to PS molecules, i.e., both electron storage and donor. This work also provides a new interpretation to explain the activation mechanism of PS. The developed CeO2-MnFe2O4 nanostructures with rapid removal efficiency, high degradation efficiency and good recyclability may provide potential guidance for the design of polymetallic oxide nanocatalysts in PS-based AOPs.

- **Keywords:** Polymetallic synergy; DFT; Magnetic catalysts; Ceria; Activation mechanism; AOPs

Daniel T. Oyekunle, Maulidi Barasa, Eman A. Gendy, Sieh Kiong Tiong. *Heterogeneous catalytic transesterification for biodiesel production: Feedstock properties, catalysts and process parameters*. Pages 844-867.

In recent years, biodiesel has attracted increasing interest as a substitute for fossil fuels. However, the cost of producing biodiesel is far greater than that of fossil fuels. As a means of reducing the cost of production, biodiesel has been produced from different kinds of feedstock based on local availability. Howbeit, the quality and efficiency of the transesterification process have been limited by the feedstock quality. It has been documented that the quality of biodiesel produced depends on the fatty acid compositions and the physicochemical properties of the oil feedstock. Moreover, the use

of heterogeneous catalysts in the trans-esterification process has been preferred due to their reusability, and ease of product separation. Different kinds of solid-based catalysts influence the yield of the biodiesel produced, this was based on the distinct basicity and textural properties of the catalyst used. Hence, researchers have sought to improve the trans-esterification reaction by altering the basicity, surface area, and porosity of the catalyst. In addition, trans-esterification process parameters such as methanol: oil ratio, catalyst loadings, reaction time, reaction temperature, stirring rate, and ultrasonic irradiation influences the catalytic transesterification reaction. Therefore, this review considers the effect of oil feedstock properties, the heterogeneous catalytic properties, and transesterification process parameters as it affects the transesterification process. It also considers the mechanism of the transesterification reaction and discusses the challenges and areas that require improvement.

- **Keywords:** Biodiesel; Feedstock properties; Heterogeneous catalyst; Catalyst properties; Transesterification reaction parameters; Energy

Zhongwen Pan, Xiaoxiang Li, Liping Fu, Qiude Li, Xinyang Li. *Environmental sustainability by a comprehensive environmental and energy comparison analysis in a wood chip and rice straw biomass-fueled multi-generation energy system*. Pages 868-879.

Biomass-based energy systems are gaining popularity as a clean and renewable source of energy, and have the potential to be a major contributor to the transition towards a sustainable energy future. In this regard, a novel multi-generation energy system is developed based on the biomass combustion. Wood chip and rice straw biomass is combusted with air agent and triggers an integrated system comprises a gas turbine cycle, a proton exchange membrane electrolyzer, a supercritical carbon dioxide Brayton cycle, and a humidification-dehumidification desalination system. The performances of wood chip and rice straw in triggering the system are compared from environmental and energy indicators viewpoints. The system fueled by wood chip emits lower carbon dioxide emission compared to the system fueled by rice straw (8.294 g/kWh compared to 10.41 g/kWh). However, the rice straw-fueled system results in higher efficiency than the wood chip-fueled system (69.9% compared to 69.1%). The system fueled by wood chip produces 2.68 kg/h of hydrogen while this value if 1.96 kg/h for the system fueled by rice straw. The research validated the possibility of utilizing energy systems that incorporate wood chip and rice straw biomass across various generations and showed the superiority of the wood chip in most cases.

- **Keywords:** Biomass; Environmental concerns; Freshwater; Hydrogen production; Biofuels

Weiye Luo, Mingshu Bi, Yue Zhang, Di Yu, Zilong Deng, Jingjie Ren. *Multi-factor coupling analysis and identification of tanks BLEVE*. Pages 880-890.

In a fire environment, liquid storage tanks are prone to integral cracking and eventually boiling liquid expanding vapor explosion (BLEVE), which a fireball, generates overpressure and ejected fragments with great impact on the safety of the tank area. Hence, it is important to reveal the influencing factors of the liquid storage tank failure process and the conditions that trigger integral cracking failure for the flammable liquid tank explosion accident prevention. This paper is aimed at the failure problem of metal storage tanks exposed to high temperature for a long time, through the fire experiment of small liquid tanks, taking the filling rate of tanks itself and the fire engulfment area as variables, the failure mechanism of tanks fire environment was explored from the aspects of pressure response, temperature response, failure form and tank deformation characteristics. A criterion was proposed to determine whether BLEVE will occur, which is

based on the comprehensive analysis of the influence of tank internal pressure and high temperature damage of the material.

- **Keywords:** BLEVE; Explosion; Pressure vessel failure; Stress rupture; Experimental results

Zhaoming Yang, Xueyi Li, Qi Xiang, Qian He, Michael H. Faber, Enrico Zio, Huai Su, Jinjun Zhang. *A resilience evaluation method of natural gas pipeline system based on uncertainty analysis*. Pages 891-908.

The natural gas pipeline system (NGPS) is a complex network of units that is susceptible to potential random failures. Moreover, the environment in which the NGPS operates is characterized by complexity and uncertainty, including market volatility, natural disasters, and deliberate sabotage. While research on the NGPS has mainly focused on supply reliability through methods such as statistical analysis and random simulation, there is a lack of emphasis on the system's supply resilience, which encompasses its robustness and recovery abilities. To address the resilience of the NGPS under uncertainty, this study proposes a probabilistic analysis model that evaluates supply resilience based on failure mechanisms and reasonable data. The model takes into account the integrated evaluation indexes framework and analyzes the process of failure and recovery, using MCMC random process analysis and complex networks theory. The results indicate that both gas transportation capacity and user satisfaction should be considered in the evaluation and strategy analysis of NGPS resilience. Furthermore, the study of resilience can provide guidance for NGPS operation, pre-warning during the design and operational stages.

- **Keywords:** Natural gas pipeline system, system resilience; Uncertainty analysis; Random process

Zhongjie Fei, SU Zhanguo, Jianbo Lu, Pradeep Kumar Singh, Mahidzal Dahari, Hasan Sh. Majdi, H. Elhosiny Ali, Souhail Mohamed Bouzgarrou. *Sustainable H2 production/separation by integration of solid oxide electrolyzer, biomass gasifier and H2 separation membrane: A techno-economic/environmental evaluation and multi-objective optimization*. Pages 909-920.

Hydrogen as a clean fuel can simultaneously respond to the challenges of energy shortage and environmental issues, provided that it is produced in a clean and cheap way. In this research, a hydrogen production system based on the combination of a solid oxide electrolyzer with a gasifier and a hydrogen separation membrane has been studied from a techno-economic outlook. In order to achieve a proper approximation of the levelized cost of hydrogen (LCOH), an elaborated economic analysis has been performed considering all aspects, where the life of the hydrogen separation membrane (HSM) and the solid oxide electrolyzer (SOE) has been taken into account. Finally, the minimization of the levelized cost of hydrogen and the levelized carbon dioxide emission (LCE) was carried out through multi-objective optimization. The cost of selling hydrogen was determined according to the various payback times. According to the conducted optimization, it is possible to obtain the minimum levelized cost of hydrogen of 3.63 $/kg. This condition leads to the levelized emission of 10.17 kg CO2/kg H2. Also, the system has the ability to bear levelized CO2 emissions up to 2.92 kg CO2/kg H2, so that the levelized cost of H2 production is 6.45 $/kg. In the four optimal conditions obtained from the optimization, considering the payback time of 5 years, the cost of selling the produced H2 can be 3.64 $/kg, 6.45 $/kg, 5.98 $/kg, and 5.29 $/kg.

- **Keywords:** Gasification; Hydrogen separation membrane; Levelized cost of hydrogen; Multi objective optimization; Solid oxide electrolyzer

Limin Kang, Jingping Liu, Yadong Yao, Xingliang Wu, Jianxin Zhang, Chen-guang Zhu, Feiyang Xu, Sen Xu. *Enhancing risk/safety management of HAN-based liquid propellant as a green space propulsion fuel: A study of its hazardous characteristics*. Pages 921-931.

The knowledge of hazard classification of hydroxylammonium nitrate (HAN)-based liquid propellant is an essential subject in prevention of safe and transportation accidents. To improve hazard classification of the propellant, various tests were conducted on both material sample and packaged sample. Differential scanning calorimeter was utilized to study thermal decomposition parameters, resulting in the determination of high values for both thermal decomposition and explosion temperatures. Koenen and EIDS gap tests were used to evaluate the heat response under high confinement and the sensitivity of shock, respectively. The results indicated that the propellant was insensitive to shock wave, with a limiting diameter of 3.0 mm. The external fire test was conducted to elucidate the explosion characteristics of the packaged propellant. Pictorial information and temperature data were recorded using high-speed camera and infrared imager. The results revealed that a mass explosion occurred during the fire process. The combination of the perforated witness screen, long-range metallic projections and high-value heat flux led to the classification of the packaged HAN-based liquid propellant as Class 1.1 C, more stringent than the traditional Class 1.3 C. The study is expected to offer valuable insights for the safety of development, preservation, and conveyance of HAN-based liquid propellant.

- **Keywords:** Hydroxylammonium nitrate; External fire test; Risk/safety management; Thermal radiation; Hazard classification

Chongchong Zhang, Boqiang Lin. *Carbon prices forecasting based on the singular spectrum analysis, feature selection, and deep learning: Toward a unified view*. Pages 932-946.

An accurate carbon price prediction is vital for governments to formulate emission reduction policies and for corporate managers to carry out sustainable management. Although many models have been proposed to meet this purpose, there is still a lack of comprehensive comparisons among the key competing models in a single study. This study conducted a comprehensive evaluation of six feature selection methods and six machine learning models for carbon price prediction, and then proposed a novel data-driven hybrid model that integrates singular spectrum analysis, random forest, and long short-term memory neural network. The results show that random forest and long short-term memory neural networks are the most competitive feature selection and prediction models, respectively. It is more reasonable to construct the model's input by comprehensively considering variables' short-, medium-, and long-term features. When the recombination value is approximately half the length of the embedding window, the singular spectrum analysis is most conducive to improving the prediction accuracy. The hybrid model proposed is always significantly superior to other benchmark models. Our work contributes to guiding carbon price modeling to help regulators and managers accurately grasp carbon price signals.

- **Keywords:** Carbon price prediction; Singular spectrum analysis; Random forest; Long short-term memory neural network

Huanxin Zhao, Xinyue Liu, Yuqi Liu, Dan Wu, Wanjie Hu, Xiaoyuan Shang, Mingyi Lv. *Directionally inducing non-radical pathways for peroxymonosulfate activation by regulating the exposed crystal plane of MnO2*. Pages 947-958.

Persulfate activation based on non-radical pathways has unique advantages in wastewater treatment. A precise design for inducing non-radical pathways by regulating the exposed crystal plane of metal oxides was proposed. Manganese dioxide (MnO2) with (310) and (110) as the main exposed planes (310-M and 110-M) were designed and synthesized for inducing different non-radical pathways. The performance of PMS activation by 310-M and 110-M for phenol degradation was investigated. The quenching experiments, EPR tests and premix experiments implied the absence of radical (SO4•- and •OH) in 310-M/PMS and 110-M/PMS systems. Combined with the results of XPS and electrochemical analysis, electron transfer process (ETP) was the dominant mechanism in the 310-M/PMS system, and Mn (III) was the active site for combining with PMS to form the MnO2-PMS* complex with strong oxidation capacity, which directly extracted the electrons from phenol. While in the 110-M/PMS system, the 1O2 oxidation pathway played a major role in phenol degradation. And the 1O2 was proved to originate from the released lattice oxygen and the single electron reduction of O2. In addition, both 310-M and 110-M exhibited high performance on phenol degradation even in the presence of inorganic ions (Cl-, NO3- and SO42-) and humic acid (HA), and showed good stability in five cycle experiments. This study highlights a novel route for precisely inducing non-radical pathways by regulating the exposed crystal planes of metal oxide catalyst on persulfate activation and improving the performance on wastewater treatment.

- **Keywords:** Peroxymonosulfate; Non-radical; MnO2; Crystal plane exposure

Le Chang, Zhixin Wu, Noradin Ghadimi. *A new biomass-based hybrid energy system integrated with a flue gas condensation process and energy storage option: An effort to mitigate environmental hazards*. Pages 959-975.

The development of biomass-fueled cogeneration plants can be fruitful to achieve the sustainable development goals, due to the crises of fossil energy-fueled ones. Additionally, biomass fuels can offer higher reliability and more sustainable energy compared to the two more well-known renewables (i.e., solar and wind energies) due to the no dependence on environmental and weather conditions. The present article provides a comprehensive assessment (thermodynamic-design, exergoeconomic and environmental) and optimization of a new biomass-driven cogeneration plant cascaded with a heat recovery unit. The planned plant is based on a biomass gasification process, some thermodynamic power generation cycles based on steam and gas turbines (i.e., Rankine cycle, Brayton cycle, and organic Rankine cycle (ORC)), and flue gas condensation process. Besides, a compressed air energy storage system (CAESS) as an energy storage process is integrated with the considered plant to establish a balance between production and demand and reduce electricity costs. To achieve optimal performance, a multi-objective optimization (based on a genetic algorithm) is applied. The findings showed that by considering the multi-objective optimization techniques, the plant's exergy efficiency could improve by about 15%. At the same time, the exergy cost rate is reduced by almost 17.3%. Avoiding the payment of carbon tax and the high electricity production level in the on-peak consumption period are unique and competitive features of the proposed biomass-driven power plant. It was also found that the LCOE and the payback period were 13.27 USD/GJ and 2.03 years, respectively, therefore, the proposed power plant exhibits reasonable economic feasibility.

- **Keywords:** Biomass energy; Flue gas condensation process; Hybrid energy system; Energy storage option; Environmental assessment; Thermoeconomic

Yang Miao, Chenghao Jia, Yang Hua, Yuejuan Li, Qingchun Tang, Jingxiang Xu, Di Wu, Xiaolu Zhang. *Simultaneous visualization of density and pressure in hydrogen leakage based on self-imaging via dual-channel interference*. Pages 976-985.

Risk assessment of hydrogen energy technologies is a necessary condition for the arrival of a hydrogen energy economy society. Currently, most methods for detecting hydrogen leaks use a single concentration or pressure sensor. Structural visualization and parametric diagnosis of complex flow fields cannot be solved simultaneously by a single detection method. The main objective of this work is to propose an advanced optical detection method to simultaneously monitor the outlet pressure and density field distribution during hydrogen leakage. For the detection of the density field distribution, we use double propagation of the laser beam in the hydrogen jet to improve the phase sensitivity and relay imaging of the object between each pass to maintain spatial resolution. Error analysis shows that the error of our proposed method is 2.47 %, which is within the error tolerance. The sensitivity analysis shows that our detection sensitivity is twice that of the conventional Mach-Zehnder interferometer. For the detection of outlet pressure, we propose a mathematical model in which the half-length axis of the laser spot is linearly related to the outlet pressure and use the deformation of the laser beam in the hydrogen jet to detect the outlet pressure. The results show that the hydrogen jet can be regarded as a gas-phase lens when detecting the outlet pressure, and the deformation of the laser beam profile in the horizontal direction increases linearly with the increase of the jet pressure. The results of the study can provide a reference for the detection of accidental hydrogen leakage and the improvement of hydrogen safety regulations.

- **Keywords:** Hydrogen safety; Density; Optical measurement; Pressure

Akif Çolak, Ali Çelik, Emre Mandev, Burak Muratçobanoğlu, Berrak Gülmüş, Faraz Afshari, Mehmet Akif Ceviz. *Study on a novel inclined solar water distillation system using thermoelectric module for condensation*. Pages 986-994.

Energy efficiency and energy conservation are critical issues today, and the use of solar energy is widely recognized as a key solution for achieving energy independence and reducing reliance on fossil fuels. In this study, a water treatment system was installed, and numerous experiments were conducted to improve energy efficiency and investigate the impact of various parameters on water distillation rates. The primary focus of this study was to increase the rate of distillation by enhancing the surface area for rapid evaporation through the use of sponge pieces, and integrating the system with a novel condensation part equipped with a mechanism that sprays water on the external heat exchanger of the thermoelectric module to increase the condensation rate. The study also examined the effects of black color on solar energy absorption, the impact of indoor fan operation on water vapor distribution, the role of insulation in reducing thermal energy losses, and the intensity of solar radiation. The results revealed that the use of sponge pieces and a thermoelectric cooler significantly increased the rate of water distillation, which was about 100.5%. Moreover, the effect of air fans on the distillation rate was observed, which increased the distillation by more than 51.1%. Overall, this study provides valuable insights into the design and optimization of solar-powered water treatment systems, highlighting the importance of energy efficiency and the potential of renewable energy sources in meeting energy needs while reducing impact on the environment.

- **Keywords:** Solar energy; Water distillation; Thermoelectric; Efficiency

Brahim Bouargane, Ilham Oubelhas, Silvia Perez Moreno, Mohamed Ghali Biyoune, Bahcine Bakiz, Juan Pedro Bolivar, Ali Atbir. *Process of preparing chloride-free KNS compound fertilizers from phosphogypsum waste using a quaternary phase diagram*. Pages 995-1005.

Phosphogypsum (PG), commonly known as calcium sulfate, is a waste by-product generated during the production of phosphoric acid by the wet phosphoric acid process (WPA). It is well known that every year the phosphate industries produce a large quantity of PG around the world (i.e., Currently, global production of this waste is estimated at 300 Mt/ year), but the valorization processes of this waste are limited and low valuable. In this study, we investigated the recycling of PG by-product, which can be considered very promising sources of sulfate ions (SO42-) for the manufacturing of chloride-free KNS compound fertilizer based on potassium-ammonium sulfate ([K1−x(NH4)x]2SO4). The primary objective of this study was to develop a methodology for [K1−x(NH4)x]2SO4 synthesis and its separation process using the quaternary phase diagram K+, NH4+ / Cl-, SO42- - H2O at 25 °C. The experiment results show that it is possible to recover relatively pure (NH4)2SO4 from PG to re-synthesize in presence of KCl the [K1−x(NH4)x]2SO4 phase, whose high quality and purity were confirmed by the combined use of several analytical and characterization techniques such as X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive X-Ray Spectroscopy (EDS), and gamma spectrometry analysis. The thermal decomposition was supplemented by Thermo-Gravimetric Analysis (TGA) coupled with Differential Thermal Analysis (DTA). The main findings of this study may assist in developing methods for valorizing PG waste by converting it into valuable fertilizer products, which are particularly suitable for cultivating chloride-sensitive crops. Thus, total or partial substitution of non-renewable resources by PG not only helps to solve the environmental pollution caused by this waste, but also reduces production costs and improves farm economics.

- **Keywords:** Chloride-free KNS; Fertilizer; Phosphate; Phosphogypsum waste; Quaternary phase diagram; Sulfates

Tao Hai, Walid El-Shafai, Riyadh AL-Obaidi, Bhupendra Singh Chauhan, Teeba Ismail Kh, Nasser M. Abd El-Salam, Babak Farhang. *The optimal design of solid oxide and molten carbonate fuel cells integration with a CO2 recycling unit: An attempt to reach a clean transition process*. Pages 1006-1018.

High-temperature Solid Oxide Fuel Cell (SOFC) technology has great potential as a clean and effective energy source. However, several issues have prevented their widespread adoption, like high operating costs, difficulty integrating with other components, and being sensitive to fuel contamination. In order to address these challenges, the main novelties of the present work are carbon capture and utilization for clean energy production, using the flue gas condensation process as a cost-effective and energy-efficient strategy, and the combination of Molten Carbonate Fuel Cells (MCFC) for increased energy efficiency and most effective component integration. The proposed novel system is also equipped with a gasifier and vanadium chloride unit for syngas and clean hydrogen production. The system's practicality is evaluated by analyzing the key performance indicators from thermodynamic, exergo-economic, exergo-environmental, and sustainability viewpoints. Also, the Sankey diagram is presented to investigate each component's effectiveness from the exergy destruction facet. According to the findings, at the most optimum design condition, the acceptable energy and exergy efficiencies of 61.06% and 50.66%, respectively, are achieved, revealing the system's effectiveness. The suggested system is also financially attractive since it achieves a reasonable levelized power cost of 17.6 $/MWh at a total cost of 44.1 $/h. The findings show that carbon dioxide recovery is crucial in reducing the pollutants due to the low emission

index of 5.01 kg/GWh. Finally, the exergo-environmental index, environmental damage effectiveness, and exergy stability factor have equivalent values of 0.012, 0.59, and 0.54.

- **Keywords:** CO2 recycle; SOFC; MCFC; Thermochemical cycle; Hydrogen; Biomass; Clean energy system

Zhaowang Dong, Bin Yang, Heng Xiong, Baoqiang Xu, Wenlong Jiang. *Decomposition behaviour of jamesonite and separating lead and antinomy sulfides via one-step vacuum distillation and multi-stage condensation*. Pages 1019-1026.

Jamesonite is known as an important complex mineral for smelting antimony. At present, the method used to separate antimony and lead by pyrometallurgy is disadvantaged by high pollution and high energy consumption. For this reason, a simple and eco-friendly method of separating antimony and lead in jamesonite from mineral source by vacuum distillation was proposed in this paper. The decomposition temperature and products of jamesonite under argon atmosphere and atmospheric pressure were determined by TG-DSC technology and variable temperature in-situ XRD detection method for the first time. The phase evolution of minerals under vacuum conditions is determined by vacuum heating method. The initial decomposition temperature of jamesonite under argon and atmospheric pressure is 583 °C, and it is basically completely decomposed above 610 °C. The intermediate products include FeSb2S4, Pb2Sb2S5, Pb9Sb22S42, Pb5Sb4S11, Fe11S12, Pb4Sb6S13, Pb12Sb10S27 etc. Under vacuum conditions, the mineral begins to decompose at 300 °C, and the temperature at the end of decomposition is about 500 °C. One-step separation of lead and antimony sulfide can be achieved by vacuum decomposition and multi-layer condensation. The lead content on the lead enrichment condensing plate is 82.78 wt%, and the antimony sulfide content of 68.18 wt% can be obtained on the antimony enrichment condensing plate.

- **Keywords:** Jamesonite; Decomposition; Vacuum distillation; Separation

Minyu He, Pengyang Zhang, Xinxi Duan, Liumei Teng, Haoyan Li, Fei Meng, Qingcai Liu, Weizao Liu. *Selective recovery of lithium from spent lithium-ion battery by an emission-free sulfation roasting strategy*. Pages 1035-1044.

As the economy recovered from the COVID-19 epidemic, the price of Li2CO3 skyrocketed to the highest. Recovery of lithium from spent lithium-ion batteries (LIBs) is significant for addressing lithium shortage and environmental issues. Sulfation roasting is often accused of being unsustainable and not environmentally friendly due to the consumption of expensive sulfation reagents and emission of SO2. Herein, a novel and green recycling process for selective separation of lithium from spent LiMn2O4 (LMO) batteries was proposed based on a SO2 emission free sulfation roasting with waste copperas. Lithium in the cathode power were selectively sulfated into soluble Li2SO4 with a conversion of 99.50%, while manganese was riched as insoluble oxides. At low temperature (e.g. 400 °C), LMO were difficult to be sulfated due to the limited sulfation ability of SO42- and mass transfer. When the roasting temperature reached 700 °C, SO2 was produced and the generated SO2 reacted in situ with the LMO to form Li2SO4 and MnSO4, preventing SO2 emissions into the atmosphere. As temperature continued to increase, the MnSO4 acted as a sulfation reagent and sulfated the unreacted LMO. All the sulfur was immigrated in Li2SO4, rather than being emitted as SO2.

- **Keywords:** Spent LiMn2O4 battery; Selectively recovery; Sulfation roasting; SO2 emission-free; Copperas

Wen-Hua Lin, Shu-Hui Liu, Chih-Yu Ma, Chi-Wen Lin. *Increased styrene vapor removal and power production by adding silicone oil to microbial fuel cell-based trickling filter.* Pages 1045-1053.

This study increases the mass transfer of hydrophobic contaminants in a microbial fuel cell-based trickling filter (MFC/TF) by adding non-aqueous phase liquid. The removal efficiency, mineralization efficiency and elimination capacity of styrene are respectively increased by 1.56 times, 1.86 times and 1.52 times, the power density is increased by 2.6 times and the internal resistance is reduced by approximately 22% after adding 10% silicone oil to the MFC/TF. This is mainly attributed to a decrease in the internal resistance after adding silicone oil, which increases electron transfer on the surface of the auxiliary anode packing and increases the number of electricity-producing bacteria. Adding 10% silicone oil to the MFC/TF increases the number of degrading bacteria and electricity-generating bacteria in the MFC/TF by 2.3–2.5 times. The performance of the MFC/TF using 10% silicone oil is significantly increased because there is increased mass transfer of styrene in the MFC/TF and increased power generation.

- **Keywords:** Hydrophobic pollutant removal; MFC; Mineralization efficiency; Bioelectricity; Microbial community

Bardia Rezvani, Seyed Reza Nabavi, Milad Ghani. *Magnetic nanohybrid derived from MIL-53(Fe) as an efficient catalyst for catalytic ozonation of cefixime and process optimization by optimal design*. Pages 1054-1071.

The catalytic activity of metal-organic frameworks (MOFs) in the degradation of environmental pollutants has garnered considerable interest recently. FTIR, FE-SEM, EDS, XRD, XPS, VSM, TEM, and N2 sorption-desorption isotherms were used to characterize Fe-based nanohybrids derived from MIL-53(Fe). In the catalytic ozonation of cefixime (CFX), the nanohybrid (CM-500) synthesized at 500 °C exhibited high efficiency. The enhanced catalytic activity of CM-500 may have been caused by Lewis acid sites (LAS), iron oxides, and oxygenated functional groups of the mesoporous carbon substrate that remained after pyrolysis of the organic framework. During 15 min of continuous ozonation, the CM-500/O3 process was the most effective at removing CFX with a removal efficiency of 97%, significantly higher than single ozonation with a degradation efficiency of 43% under the same conditions. Modeling and optimization of process conditions were conducted using a novel and efficient class of experimental design, namely optimal design with the fewest possible runs. Calculated CFX degradation kinetic rate constants were 0.212 min-1 with CM-500, 0.043 min-1 with MIL-53 (Fe), and 0.038 min-1 for ozonation alone. Mineralization (measured COD and TOC) is significantly higher in the CM-500/O3 system compared to single ozonation. Moreover, the scavenging experiment confirmed that the reactive oxygen species in the catalytic ozonation of CFX are surface-adsorbed superoxide and hydroxyl radicals. Due to CM-500's sustained activity and magnetic properties, it is expected that it has a high catalytic capacity for treating pharmaceutical wastewater.

- **Keywords:** Metal-organic framework; MIL-53(Fe); Magnetic nanohybrid; Fe-based catalyst; Catalytic ozonation; Cefixime; Optimal design

Zhongwei Meng, Jingtong Zhang, Zhongqiang Bao, Wei Wang, Huan Deng, Yizhang Hu. *Numerical simulation of diesel particulate filter performance optimization through pore structure analysis*. Pages 1072-1084.

Based on the theory of spherical filled bed, the internal porous media filter wall of the Diesel Particle Filter (DPF) is assumed to fill the filter wall of the unit cell. Since particle

trapping by DPF is a dynamic process, the particle deposition characteristics inside DPF are simulated by numerical simulation in this paper. The influence of macroscopic incoming flow parameters and microstructural parameters on DPF filtration performance is investigated, and then the optimization window that can improve DPF filtration performance is explored. The results show that increasing the exhaust temperature and incoming particle concentration leads to an increase in the filtration efficiency and pressure drop of DPF, while the higher the filtration velocity, the lower the filtration efficiency of DPF. In addition, the larger the porosity, the higher the filtration efficiency and pressure drop of DPF, while the increase in the average pore size and pore size distribution range leads to a decrease of the filtration performance of DPF. On this basis, evaluation indexes that can evaluate the filtration performance of DPF are proposed to provide a theoretical basis for optimizing the substrate parameters of DPF.

- **Keywords:** Diesel Particulate Filter; Porous Media; Unit Cell; Optimization; Filtration Efficiency; Pressure Drop

Yongkui Li, Xiaodong Pan, Suqin Li, Xin Zhao, Penghui Guo, Tao He. *Innovative technology for preparation of high-purity silica from vein quartz ore through S-HGMS coupling acid leaching process*. Pages 1103-1115.

In the present work, an S-HGMS coupling acid leaching technology was established to prepare high-purity silica using vein quartz ore. Firstly, the magnetic properties of different phases in vein quartz were investigated through density functional theory (DFT) calculations and arranged the phases in terms of magnetic susceptibility: FeP2 > Al2SiO5 > SiO2 > Ca(Al2Si2)O8 > AlPO4. Those differences in magnetic susceptibility resulted from the spin state of electrons in the ions. After treatment using the S-HGMS process, weakly magnetic particles are effectively separated from silica particles, and the obtained silica concentrate contained SiO2 of 99.690% purity. Subsequently, lattice impurity ions were removed through a fluorine-free and low-fluoric acid leaching process. Under optimal conditions, the SiO2 purity in high-purity silica reached 99.954% and 99.990% in the two processes. The lattice parameters and volume of α-quartz in high-purity silica obtained with low-fluoric acid leaching were less than those obtained with fluorine-free acid leaching. This difference can be attributed to the reaction between HF molecules and lattice impurity ions, resulting in the generation of coordination compounds. Meanwhile, HF dissolved SiO2 and opened the lattice impurity ions channel, promoting lattice impurity ions depth removal. This study established a complete set of critical technologies for preparing high-purity silica from vein quartz through the S-HGMS coupling acid leaching process, providing theoretical and scientific bases for industrial applications.

- **Keywords:** High-purity silica; Vein quartz ore; S-HGMS; Acid leaching; Lattice impurity ions

Nan Chen, Hang Yao, Xinyi Liu, Juncheng Jiang, Lei Ni. *Investigation of the thermal hazard and decomposition mechanism of 1,1-di(tert-butylperoxy) cyclohexane by experiment and DFT simulation*. Pages 1116-1128.

1,1-Di (tert-butylperoxy) cyclohexane (1, 1-DTBCH), as an important organic peroxide, is commonly used as initiator, curing agent and crosslinking agent in the chemical industry. Due to the presence of peroxy bonds, the thermal instability of 1, 1-DTBCH may incur a decomposition reaction and cause further thermal runaway. The thermal decomposition characteristics and runaway reaction characteristics of 1, 1-DTBCH were investigated by differential scanning calorimetry (DSC) and accelerated rate calorimetry (ARC). The kinetic triplet and thermal safety parameters were calculated by using non-isothermal

method. The gaseous products and pyrolysis products of 1, 1-DTBCH was investigated by thermogravimetric and infrared spectroscopy (TG-FTIR) and gas chromatography/mass spectrometry (GC/MS). The thermal decomposition pathway of 1, 1-DTBCH was explored with density functional theory (DFT). The exothermic dominant reaction in the thermal decomposition process of 1, 1-DTBCH was explored by combining experiment and theoretical calculation. The corresponding safety control measures were provided to reduce the thermal runaway hazard of 1, 1-DTBCH.

- **Keywords:** Thermal runaway; Thermal decomposition characteristics; Thermal safety parameters; Density functional theory; Thermal decomposition pathway

Saeed Fallah Ahmadi, Asgar Minaei, Mohammad Ebadollahi, Hadi Ghaebi, Mahsa Hasanzadeh Shahrivar. *Energy management and reducing the environmental impacts of industrial flare gases using a new trigeneration energy system*. Pages 1129-1141.

Recovering the heat of flare gases through energy systems exploits a waste source of energy and contributes to the industrial development of societies. Reducing environmental pollution and energy management of flare gases are considered among the main necessities of industrial complexes, especially refineries. One of the methods to reuse these gases is to employ them in downstream energy systems to produce useful products. A novel trigeneration energy system is presented for power, heating, and freshwater production by recovering the waste heat of industrial flare gases. The system is scrutinized from thermodynamic and thermoeconomic criteria. Furthermore, a multi-objective optimization of the set-up is performed. Optimization results show an acceptable increase in energy and exergy efficiencies while a decrease in the unit cost of product is obtained.

- **Keywords:** Flare gases; Cogeneration system; Sustainability; Environmental pollution; Energy and exergy analysis; Thermoeconomic

Longguang Peng, Jicheng Zhang, Shengqing Lu, Yuanqi Li, Guofeng Du. *One-dimensional residual convolutional neural network and percussion-based method for pipeline leakage and water deposit detection*. Pages 1142-1153.

Pipeline leakage and water deposits can cause serious consequences, such as environmental pollution, safety accidents, and economic losses. Therefore, effective detection of these flaws is of critical importance. Currently, most of the detection methods rely heavily on experienced inspectors and specialized equipment, which is labor-intensive and costly. To this end, this paper presents a one-dimensional residual convolutional neural network (1D-ResNet) based percussion method, for detecting pipeline leakage and water deposit. The proposed method uses sound produced by tapping the pipe as input to 1D-ResNet, which can directly extract features from the audio signal, avoiding hand-crafted feature extraction process. The effectiveness of the proposed method is validated through experiments, showing strong performance in pipeline fault detection. Furthermore, the 1D-ResNet method exhibits better classification performance and stronger noise robustness compared to other methods. In summary, this study presents a novel approach for the detection of pipeline leakage and deposit through the innovative introduction of 1D-ResNet deep learning technology, which has significant application prospects.

- **Keywords:** Leakage and deposit detection; Percussion-based method; One-dimensional residual convolutional neural network; Residual block; Automated pipeline detection

Miao Mou, Xiaoqiang Zhao, Kai Liu, Yongyong Hui. *Variational autoencoder based on distributional semantic embedding and cross-modal reconstruction for generalized zero-shot fault diagnosis of industrial processes*. Pages 1154-1167.

The traditional fault diagnosis models cannot achieve good fault diagnosis accuracy when a new unseen fault class appears in the test set, but there is no training sample of this fault in the training set. To solve this problem, a generalized zero-shot fault diagnosis model for industrial processes based on distributional semantic embedding and cross-modal reconstruction variational autoencoder (DSECMR-VAE) is proposed. DSECMR-VAE uses two variational autocoders (VAEs) to encode the features from two different modalities of fault samples and fault attribute semantic vectors into latent variables, and then uses the latent variables to generate fault samples belonging to the seen and unseen fault classes. In addition, a Barlow matrix is designed specifically for the distribution parameters of the latent variables, this matrix is utilized to measure the consistency between the distribution of fault samples and fault attribute semantic vectors. Subsequently, cross-modal reconstruction is performed on VAE. Cross-modal reconstruction uses the input from different modalities to reconstruct the current input, which can fully combine the information from different modalities. Finally, a classifier is trained based on the obtained latent variables to realize the generalized zero-shot fault diagnosis. Two case studies demonstrate the effectiveness and superiority of the proposed model for zero-shot and generalized zero-shot fault diagnosis.

- **Keywords:** Fault diagnosis; Generalized zero-shot learning; Variational autoencoder; Attribute semantic description; Distributional embedding; Cross reconstruction

Fusong Wang, Xiaoqing Li, Shaopeng Wu, Lifei Zheng, Qiuyuan Luo, Jixin Zhang, Diego Maria Barbieri. *Comparative study for global warming potentials of Chinese and Norwegian roads with life cycle assessment*. Pages 1168-1180.

Mitigation of GHG emission is increasing concerned in the research field of road engineering. The quantitative assessments of integral road structural designs in different countries would shed light on the implementation of sustainable road development and global warming controlling. The study referred to the European E6 and the Yanqing-Chongli expressway to quantify the GHG emissions for Norwegian and Chinese roads, and investigate the critical procedures and factors in resulting in the differences of GHG emissions. The data inventory and research framework for life cycle assessment (LCA) were established according to their applied materials, structural design and construction techniques. Moreover, the quantification of GHG emission was conducted as considering the surface layers, base layers, subbase and frost protection layer. The comparative results indicate that the Norwegian road generated extra 1.43 t equivalent CO2 more than Chinese road during the 20-year service life, and the surface layers are the most source of GHG emission in road structure, which occupied 65.75% for Chinese road and 43.19% for Norwegian road. Additionally, the materials extraction phase caused the largest proportion of GHG emission in Chinese road case, while the road construction phase was verified as the capital GHG contributor in Norwegian road case with 108.27 t equivalent CO2 emitted. The obtained results in the comparative study could provide the practical references for low-carbon road construction and promising strategies for globalization development.

- **Keywords:** Road construction; GHG emission; Life cycle assessment; Road structural design; Global warming controlling

A.J. Nakhal A., R. Patriarca, F. De Carlo, L. Leoni. *A System-Theoretic Fuzzy Analysis (STheFA) for systemic safety assessment*. Pages 1181-1196.

The interactions among distinct systems and components have attracted more attention recently due to safety concerns. Indeed, modern industrial plants could be regarded as complex socio-technical systems influenced by human, social, and organizational aspects. To model this level of complexity, System Theory (ST) and related frameworks, such as System-Theoretic Accident Model and Processes (STAMP) have been introduced. Despite their strengths and abilities, ST techniques are mainly qualitative and provide much information, eventually complicated to analyse and summarize. Fuzzy Set Theory (FST) and expert elicitation could be employed to cope with the former challenges. However, addressing the uncertainty arising from differences in expert opinions is necessary. To this end, this paper aims to develop a framework to conduct system safety assessments based on the integration of STAMP and FST. In this context, an improved version of the Similarity Aggregation Method is adopted to aggregate judgments. To demonstrate the application of the approach, a Natural Gas Regulating and Metering Station (NGRMS) is considered as the case study. The results show that the methodology is able to provide quantitative information by associating a level of criticality with each control action. Accordingly, managers could exploit the framework to identify priorities for directing efforts.

- **Keywords:** System thinking; Industrial accident analysis; Fuzzy logic; STAMP model; Expert opinion

Kun Xu, Shuang Li, Cheng Lu, Jiao Liu. *Risk assessment of coal mine gas explosion based on cloud integrated similarity and fuzzy DEMATEL*. Pages 1211-1224.

The risk of coal mine gas explosion seriously threatens the continuous safe production of coal mines, which in turn affects the national energy security, so it is important to prevent and control the coal mine gas risk. Current risk assessment methods are difficult to fully express the uncertainty in the assessment process, and calculating index weights is easy to deviate from reality. This study introduces Decision-making Trial and Evaluation Laboratory (DEMATEL) as well as the cloud model, and proposes a new coal mine gas explosion risk assessment model based on cloud integrated similarity and fuzzy DEMATEL. The model fully expresses the uncertainty in the whole risk assessment process and makes the index weights assignment more reasonable. It also combines the calculation of cloud integrated similarity to more accurately determine the risk level based on the advantage that the cloud model can visually display the risk status of the assessment object. An example study was conducted on a mine of a large state-owned coal mine enterprise in Shaanxi Province, China. The results show that the method helps coal mine enterprises to accurately assess gas explosion risks, identify weak links in risk prevention and control, and provide a powerful means for continuous improvement of risk management level.

- **Keywords:** Coal mine; Gas explosion; Risk assessment; DEMATEL; Cloud model

Krishnamoorthy Ramalingam, Elumalai Perumal Venkatesan, Suresh Vellaiyan, Azfarizal Mukhtar, Mohsen Sharifpur, Ahmad Shah Hizam Md Yasir, C Ahamed Saleel. *Substitution of diesel fuel in conventional compression ignition engine with waste biomass-based fuel and its validation using artificial neural networks*. Pages 1234-1248.

This study aims to derive bioenergy from waste lather fat and citronella grass. Lather fat oil (LFO), citronella grass oil (CGO), a mixture of leather fat oil and citronella grass oil

(LFCGO), and a nano-additive-incorporated mixture of lather fat oil and citronella grass oil (NFCO) were synthesized and used in diesel engines as the novelty of this study. ASTM standards were used to investigate and guarantee the fuel's properties. According to the experimental report, the nanoadditive's brake thermal efficiency and brake-specific fuel consumption were more comparable to diesel fuel. Compared to diesel, the NFCO blend reduced hydrocarbon, carbon monoxide, and particulate emissions by 6.48%, 12.33%, and 16.66%, respectively, while carbon dioxide and oxides of nitrogen emissions increased. The experiment's outcomes were verified using an artificial neural network (ANN). The trained model exhibits a remarkable coefficient of determination of 98%, with high R values varying from 0.9075 to 0.9998 and low mean absolute percentage error values ranging from 0.97% to 4.24%. Based on the experimental findings and validation report, it can be concluded that NFCO is an efficient diesel fuel substitute.

- **Keywords:** Waste to energy; Nano additive; Peel oil; Lather fat oil; NOx emission

Leticia Mirella da Silva, Ismael F. Mena, Miguel A. Montiel, Cristina Saez, Artur J. Motheo, Manuel A. Rodrigo. *Electrochemical generation of chlorine dioxide for use in environmental remediation*. Pages 1249-1259.

This work focuses on the production, in continuous mode, of chlorate and hydrogen peroxide, using tailored electrochemical cells specially designed to obtain high efficiencies in these electrochemical processes. Then, these chlorate and hydrogen peroxide electrochemically produced were mixed for the chemical formation of chlorine dioxide, susceptible to be used for environmental applications. In this work, not only the prototype's conceptualization, design, and 3-D printing manufacturing are realized, but also the characterization of the cells in terms of fluid dynamics, mass transfer, and production of the target compounds is made. The chlorate prototype, with an electrode area of 78.5 cm2, produced up to 1200 mg h−1 of a chlorate solution with a purity of 50 %. The hydrogen peroxide prototype, with an electrode surface area of 10.9 cm2, produced up to 9 mg h−1 of hydrogen peroxide with a concentration of up to 70 mg L−1. The chlorine dioxide was produced continuously with these compounds (HClO3 and H2O2), operating at low H2O2/HClO3 ratios and with a highly acidic supporting media. The oxidant was effectively transferred to a gaseous stream through air stripping. It was then introduced to solutions containing iodine or methomyl to confirm its ability to oxidize substances and to assess its potential use for environmental applications. These findings indicate that using Gaseous Oxidants Mediated Electrochemical Technology (GOMET) with chlorine dioxide is a viable solution for environmental remediation, offering promising prospects for future research on this topic.

- **Keywords:** Chlorine dioxide; Continuous production; Chlorate; Hydrogen peroxide; Remediation

Gleilson de F. Vieira, Inalmar D. Barbosa Segundo, José Eudes L. Santos, Amanda D. Gondim, Elisama V. dos Santos, Carlos A. Martínez-Huitle. *Electro-oxidation of wastewater from a beauty salon: The influence of electrolyte type in the removal of organic load and energy consumption*. Pages 1260-1271.

The aim to ensure water quality and wastewater treatment is sought by the United Nations and expressly proposed in the sixth sustainable development goal (SDG6). As universally available services, beauty salons (BS) are places that deal with potentially hazardous chemicals, and their effluent should be treated before goes to the sewage system. This work presents a wide characterization of a BS effluent and its respective electrochemical treatment by using boron-doped diamond (BDD) as the anode, stainless steel as the cathode, as well as NaCl and Na2SO4 as additional supporting electrolytes.

The effectiveness of the processes and the comparative study of the performance of the electrolytes were mainly performed by the analysis of chemical oxygen demand (COD) removal and energy consumption. However, other parameters were taken into consideration, such as color, conductivity/salinity, pH, and more extensive analysis regarding the cause of turbidity and the appearance of a precipitate before and during the electrolysis. NaCl proved to be more efficient than Na2SO4 to treat this BS effluent; it was not only because achieves a better COD removal (70% against 64%, with a current density of 10 mA cm−2), but also because it promoted an effluent with less turbidity and color, besides a pH closer to neutral, with no need to further correction before discharge. Regarding the electrolyte concentration, the excess of salt proved to be necessary to promote a higher removal rate in COD values with less charge and energy consumption. Thus, the concentration of 0.16 M of NaCl associated with a current density of 10 mA cm−2 was chosen as the best condition for treating this effluent. In addition, Si-based oxides were detected in the raw effluent and these were pointed out as responsible for its high turbidity. Proper discharge of it into the sewage system is reached with NaCl as the electrolyte. The treatment proposed in this work deals with SDG6 and can be used as an alternative to decision-makers and governments to help in the implementation of better politics of water sanitation.

- **Keywords:** Beauty salon effluent; Electro-oxidation; Precipitates analysis; High-turbidity wastewater; Silicates; diamond electrode

Md. Abdul Moktadir, Jingzheng Ren. *Tannery solid waste valorization for achieving SDGs: An innovative decision-making model for critical success factors analysis and sustainable technology selection*. Pages 1272-1293.

Sustainable tannery solid waste (TSW) management is essential for achieving several sustainable development goals (SDGs) and promoting carbon neutrality in the leather processing industry. However, the sustainable management of TSW in developing countries remains a relatively ambiguous and unexplored area in the research. To expedite the sustainable management of TSW, it is essential to conduct a comprehensive study of critical success factors (CSFs) and valorization technologies considering the uncertainties involved as TSWs are major contributors to environmental pollution and carbon emissions. Unfortunately, existing models are unable to effectively handle uncertainty on a broader scale when evaluating interdependencies and valorization technologies. Therefore, this study proposes a novel integrated model that combines Interval Type-2 Trapezoidal Fuzzy Sets (IT2TrFSs) based Delphi technique, an extended version of the Weighted Influence Non-linear Gauge System (WINGS) method, and IT2TrFSs- Combined Compromise Solution (CoCoSo). This model is then applied to assess the interdependencies among CSFs and TSW valorization technology using a real case study. The IT2TrFSs-WINGS analysis reveals that "Environmental policies for TSW management" is the most crucial causal CSF, with a value of 0.00560. The IT2TrFSs-CoCoSo analysis confirms that "Gasification" is the most promising TSW valorization technology, receiving a significant preference value of 2.03982. These findings will enable decision-makers, relevant stakeholders, and environmental agencies to take necessary actions towards improving the TSW management process in developing countries.

- **Keywords:** Waste-to-energy; Tannery solid waste valorization; Carbon neutrality; Solid waste management; IT2TrFS; Interval Type-2 Trapezoidal Fuzzy Sets-Delphi; Weighted Influence Non-linear Gauge System; Combined compromise solution

Guihua Bo, Fengxiang Li, Bhupendra Singh Chauhan, Hadi Ghaebi. *Multi-objective optimization and 4E analyses to simultaneous production of electricity, freshwater, H2 and cooling based on biogas-steam reforming*. Pages 1307-1320.

In the current study, a state-of-art biogas-driven poly-generation power plant is presented, evaluated and optimized. For assessing the multi-aspects feasibility of the proposed plant, exergy, energy, exergoeconomic, and environmental evaluations are applied as the robust tolls to the assessment of the plant. Also, to enhance the hydrogen production by the system, the steam reforming technology and proton exchange membrane are incorporated into the plant. Based on the obtained results, the designed plant can generate 86.04 kW, 0.9662 kg/s, 958.2 kW, and 704.573 kg/h of electricity, fresh water, cooling, and hydrogen, respectively. In this plant, the energy efficiency is approximately 33.5%, while the exergy efficiency is about 31.2%. Also, some unit cost of the product and environmental penalty cost rate are calculated at about 23.7 $/GJ and 141.7 $/h. Analyzing sensitivity helps identify which parameters affect the system's performance and determine the most effective optimization mode. The multi-objective optimization mode result improves the exergy and energy efficiencies of the plant by 19.9% and 24.5%, respectively.

- **Keywords:** Biogas; Multi-generation; Hydrogen; Desalination; Optimization

Fulai Liu, Muhammad Asadollahzadeh, Bhupendra Singh Chauhan, Ibrahim Elbadawy, Mohamed Abouelela, Bashir Salah, Huynh Nháng. *Exergoeconomic and environmental analyses of a geothermal-powered tri-generation system: A study of CO2 emission reduction*. Pages 1321-1335.

A geothermal-powered tri-generation system is presented and discussed from thermodynamic, exergoeconomic, payback period, extended-environmental, and exergoenvironmental perspectives. The designed system consists of an organic flash cycle assisted by a two-phase ejector and a vapor compression cycle that utilizes a zeotropic working fluid of Isobutane/Pentane. To further recover waste heat, an electrolyzer unit is utilized as a subsystem for producing H2. All the system outputs except for the exergoenvironmental index and exergoeconomic factor reach the highest point when the mass fraction of Pentane increases. According to a parametric study, the greatest variations in system products are related to changes in the flash tank temperature. Furthermore, the system outputs indicate a non-linear relationship with the mass fraction of Pentane. The temperature of evaporators has a substantial influence on the system's cooling capacity. Meanwhile, the remaining output parameters remain steady or show minor changes. By increasing the flash tank temperature, the costs related to electricity, cooling, and H2 all decreased before gradually increasing. The two-phase ejector has the highest exergy destruction rate because of the energy lost in the mixing process.

- **Keywords:** CO2 emission; Exhaustive study; Exergoeconomic; Environmental effects; Tri-generation

Aisvarya Srinivasan, Kalyanasundaram Manickavasagam, Kannan Malaichamy, Lakshmanan Arunachalam, Preetha Sundaram, Elango Kolanthasamy, Govindaraju Kasivelu. *Impact of silver nanoparticles against stored product pest Sitophilus oryzae (L.) and effect on agromorphological characteristics of Zea mays (maize seeds)*. Pages 1336-1350.

The present study, comparative entomotoxic efficacy of silver nanoparticles obtained through the chemical and biological route against Sitophilus oryzae L. Physicochemical characterization results revealed that silver nanoparticles (Ag NPs) were spherical morphology with an average size of 20–51 nm having excellent stability. XRD diffraction peaks showed major peaks at (2 theta) 38.19º, 44.37º, 64.56º, and 77.47º confirming their crystalline nature. UV–vis spectra inferred strong absorbance between 410 and 450 nm. Bioassay studies exhibited the LD50 values as 40.16 mg/100 g for c-Ag NPs and 24.69 mg/100 g for b-Ag NPs. The mortality brought by b-Ag NPs at the dose of 130 mg after 6 days of exposure was 100% whereas only 80% of mortality was observed for c-Ag NPs at the same dose. These c-Ag NPs also enhanced seedling characteristics i.e., germination (96%), seedling length (45.33 cm), vigor index (4351.68), and dry matter production (4.20 g). The experiment results shows that the b-Ag NPs are an alternative to insecticides against S. oryzae and improving agromorphological characteristics of maize.

- **Keywords:** Silver nanoparticles; Toxicity; Sitophilus oryzae; Maize seed; Agromorphology

Mitchell Huffman, Qingsheng Wang, Faisal Khan. *Analysis of sustainability metrics from a process design and operation perspective.* Pages 1351-1365.

As the human population grows, the strain on resources and the environment grows exponentially. Sustainable practices are therefore necessary to protect the planet as well as preserve the standard of living of those inhabiting it. The quantification of sustainability is vital to monitor and regulate industry practices. Therefore, it is necessary to understand the development of the field of sustainability quantification. Frameworks such as life cycle assessment, impact assessment, and the triple bottom line provide approaches to quantify, understand, and implement sustainability concepts. Many studies have expanded on these frameworks to provide a variety of methods to quantify sustainability in industry, with various strengths and weaknesses. Sustainability metrics to this point have lacked an inclusion of safety, time dependence, and quantification of the interrelations between sustainability pillars. To determine the validity of existing metrics, the consistency of their results must be compared. When utilizing existing sustainability indices, significant variation was found both in the final quantification of sustainability for a single process, and in the determination of a more sustainable process when comparing two processes. These inconsistencies imply the need for additional considerations within the various indices. Therefore, an interrelated, time dependent quadruple bottom line is necessary to provide a thorough assessment of the sustainability of a process.

- **Keywords:** Process system sustainability; Sustainability metric; System safety; Safety assessment

Yipeng Wu, Xingke Ma, Guancheng Guo, Yujun Huang, Mingyang Liu, Shuming Liu, Juan Zhang, Jingjing Fan. *Hybrid method for enhancing acoustic leak detection in water distribution systems: Integration of handcrafted features and deep learning approaches*. Pages 1366-1376.

Leak detection of water pipelines is of great significance to ensure water supply safety and conserve water resources. In the context of the prevalence of deep learning which can automatically extract features, deep learning-based acoustic leak detection methods are flourishing. The study compares the deep learning methods and traditional machine learning methods which need human-involved feature engineering, from aspects of detection performance, data requirement, and computational complexity. Furthermore, a hybrid leak detection method that integrates handcrafted features into deep learning networks is proposed. In this study, there are 70 features extracted from acoustic signals, constructing an extreme gradient boosting (XGBoost) classifier. Then three commonly used deep learning classifiers and the hybrid classifier are developed to carry out comparisons. Results show that handcrafted features, especially linear prediction features, still play an important role in acoustic leak detection at the current stage. The XGBoost classifier with key features can outperform deep learning classifiers and achieve acceptable computational complexity. Limited by insufficient data, deep learning classifiers cannot fully exploit their ability to directly extract useful features from model inputs (e.g., acoustic signals' waveforms in the time or frequency domain). The hybrid classifier, requiring neither careful selection of handcrafted features nor complex deep learning network structures, obtains the best detection performance using the same amount of data, showing great promise in practical applications.

- **Keywords:** Acoustic leak detection; Water pipeline; Feature engineering; Extreme gradient boosting; Convolutional neural network; Water distribution system

Nuhindro Priagung Widodo, Septian Hadi Putra, Ahmad Ihsan, Rudy Sayoga Gautama, Jianwei Cheng, Fadli Zaka Waly, Dimas Agung Permadi. *The study of coal dust minimum explosion concentration of subbituminous coal*. Pages 1387-1392.

The coal dust explosion tests have been conducted using an explosion chamber 20-L with coal dust sizes of 53–44 μm (average particle size is 48.5 μm) for subbituminous coal from Indonesia. The coal dust explosion has been tested with various energies of the ignitor, i.e., 4.2 kJ, 6.3 kJ, and 8.4 kJ, to obtain the effect of ignitor energy on the coal dust's Minimum Explosion Concentration (MEC). The results show that the MEC for the 4.2 kJ, 6.3 kJ, and 8.4 kJ ignitor energy are 120 g/m3, 100 g/m3, and 70 g/m3, respectively. The present study in subbituminous coal resulted in a relatively higher MEC compared to previous studies conducted in bituminous coal.

- **Keywords:** Coal Dust Explosion; Minimum Explosion Concentration; Explosion Chamber; Ignitor Energy

Yin Lv, Lang Liu, Pan Yang, Geng Xie, Caixin Zhang, Shunchun Deng. *Study on leaching and curing mechanism of heavy metals in magnesium coal based backfill materials*. Pages 1393-1402.

In order to promote the resource utilization of bulk solid waste, it is an effective way to improve the comprehensive utilization level of solid waste and alleviate the environmental pressure caused by storage by using all solid waste as raw material for backfill cementing. In this paper, a magnesium coal based backfill material (MCB) with modified magnesium slag (MMS) and fly ash (FA) as cementing agents, coal gasification coarse slag (CGCS) and coal gangue (CG) as aggregates was proposed. First, the mechanical properties of MCB were studied and then the hydration effect was verified

microscopically. Then, the leaching characteristics of raw materials CGCS, CG, and backfill material MCB were characterized. Furthermore, the mechanism of heavy metal leaching and solidifying of MCB was revealed by studying As and Pb. The results show that: (1) The addition of a suitable amount of CGCS with potential pozzolanic activity produces more MCB hydration products such as C-S-H and AFt with a high CG-CGCS ratio. The compressive strength reaches the maximum value of 10.21 MPa when the curing time is 28 days and the CG-CGCS ratio is 3:1. (2) The leaching levels of the target elements (As, Pb, Cr, Mn, Zn, Cu, Cd, Hg, Ag) of CG meet the limits of the class III groundwater quality standard (III-GQSL) in GB/T 14848–2017. The concentration of Pb in CGCS is 12 μg/L, which exceeds the III-GQSL limit of 10 μg/L. The overall leaching risk is CGCS>CG. (3) MCB has a good stabilization/solidification effect on the heavy metal elements Cd, As, and Pb in raw materials. The heavy metal leaching results of MCB with a low CG-CGCS ratio meet the limit of III-GQSL, and the environmental leaching risk is low. (4) In addition to physical encapsulation, the main curing mechanisms of MCB include chemical bonding, alkaline environment, and adsorption. MCB can be used as a potential consolidation agent for the solidification of heavy metal elements. While having good mechanical properties, it can also treat solid waste and effectively stabilize/solidify toxic elements in materials and has the potential for safe application in backfill.

- **Keywords:** Coal gasification coarse slag; Solid waste backfill; Leaching toxicity; Stabilization/solidification

Abdul Samad, Iftikhar Ahmad, Manabu Kano, Hakan Caliskan. *Prediction and optimization of exergetic efficiency of reactive units of a petroleum refinery under uncertainty through artificial neural network-based surrogate modeling*. Pages 1403-1414.

Process uncertainties have been a big challenge to the stable operation and control of process industries. The current study is based on the use of an artificial intelligence model as a surrogate in the online optimization of process conditions of reactive units of a petroleum refinery under uncertainty. Initially, a steady-state Aspen model was used to perform exergy analysis for quantifying the exergy efficiency, irreversibility, and improvement potential of the plant. The process model was then transformed to a dynamic mode by inserting ±5 % uncertainty in process conditions, i.e., mass flow rate, pressure, and temperature, to generate a dataset of 216 samples. An artificial neural network (ANN) model was developed using the dataset to predict exergy efficiency. The ANN model was used as a surrogate in GA and PSO environments to achieve higher exergy efficiency under uncertainty. The optimized process condition derived through GA and PSO based approaches were fed to Aspen model for cross-validation. The Fourier Amplitude Sensitivity Test (FAST) was performed to identify the most influential process conditions in terms of their effect on process exergy efficiency. The overall plant had an exergy efficiency, irreversibility, and improvement potential of 50.57 %, 34,955.55 kW, and 17,276.98 kW, respectively. The correlation coefficient of ANN model was 0.97432. The use of ANN as a surrogate in the optimization frameworks outperformed the standalone (SA) Aspen model of the process in attaining the highest exergy efficiency. Overall the performance of both the GA and the PSO based approaches were comparable. Based on sensitivity analysis, inlet temperatures of reactors were the most sensitive variables affecting the process exergy efficiency. The current study helps in laying a foundation for the simulation of Refinery 4.0.

- **Keywords:** Genetic algorithm; Particle swarm optimization; Exergy efficiency; Exergy destruction; Energy recovery; Machine learning

Keyang Liu, Baoping Cai, Qibing Wu, Mingxin Chen, Chao Yang, Javed Akbar Khan, Chenyushu Wang, Hasini Vidumini Weerawarna Pattiyakumbura, Weifeng Ge, Yonghong Liu. *Risk identification and assessment methods of offshore platform equipment and operations*. Pages 1415-1430.

Risk management is crucial for the safety of offshore platforms. With advancements in safety management, much data on hidden dangers has been generated. The data contains a wealth of risk information, which realistically reflects the current state of safety on offshore platforms. However, this data is unstructured natural language, which cannot be analyzed statistically or queried with structured fields. Moreover, the manual identification of risk factors from hidden danger data is time-consuming and subject to subjective biases. A method for risk identification and assessment for offshore platform equipment and operations based on text mining of hidden danger data is proposed. From a big data perspective, a framework for expressing risk factors is established, which completes the transition from an unstructured text about the hidden danger to a structured expression of risk information. An automated method for risk identification is developed that combines machine learning, deep learning, and natural language processing techniques. The identified risk factors are used to build the Bayesian network model for data-driven risk assessment. Data from China's Bohai oil field is used to demonstrate the effectiveness of this method. The result shows that it improves the identification of risk factors and the automation of the assessment.

- **Keywords:** Risk factors identification; Text mining; Risk assessment; Bayesian Networks

Jinlong Zhao, Qingyuan Zhang, Zhenhua Wang, Rui Yang, Jianping Zhang. *Continuous boilover behaviors of large-scale kerosene pool fires under sub-atmospheric pressure*. Pages 1431-1439.

Accidental fire is a major safety concern in chemical parks, highlighted by the several major fire accidents involving storage tanks in recent years. Boilover is considered as one of the most destructive tank fire scenarios, which occurs when a liquid fuel burning on a water layer, leading to the explosive evaporation of water and consequently a sudden increase of the heat release rate (HRR) and associated flame height due to the splashing of burning fuel. Previous studies on boilover with large-scale pool fires were mostly conducted under normal atmospheric pressure. However, chemical parks are often located in plateau regions, where the effects of reduced pressure on boilover behaviors were rarely examined. Moreover, following the initial boilover, continuous boilover could occur, and its understanding is particularly important in the thermal hazard and risk analysis and firefighting of tank fires. In this study, thin-layer boilover experiments were conducted under sub-atmospheric pressure using aviation kerosene (RP-3) with various initial fuel thicknesses and pool diameters. The burning process, boilover intensity, temperature in the fuel and water layers and associated thermal hazard were analyzed. Experimental results showed that continuous boilover occurred in all test conditions, characterized by a high intensity initial boilover followed by a series of subsequent ones with gradually reduced intensity. The mass burning rate and flame height varied significantly during boilover. It was found that the boilover intensity increases with the initial fuel thickness but decreases with the pool diameter and approaches a nearly constant value when the pan diameter is sufficiently large. The temperature at the fuel/water interface was found to increase from 93 ℃ to around 108 ℃ during boilover, both of which are lower than those observed under normal atmospheric pressure due to reduced water boiling point. The thermal hazard calculated for the initial boilover is highest as expected, and that of subsequent boilovers gradually decreases but could still be higher than that at the steady burning stage. The findings in this work will contribute to risk assessment of continuous boilover in fire accidents.

- **Keywords:** Thin-layer boilover; Large-scale pool fires; Sub-atmospheric pressure, boilover intensity; Interface temperature; Thermal hazard

Wenyi Sun, Yi Pan, Zhen Pan, Liyan Shang, Li Zhou, Zhenbo Lv. *Comparative analysis of two cogeneration systems with different connection modes*. Pages 1440-1460.

This study explores the differences between two novel cogeneration systems with different connection modes. These two systems are the series and parallel systems composed of the Brayton cycle, the organic flash cycle, and the organic Rankine cycle, respectively, which both recover flue gas waste heat and LNG cold energy. First, the equipment and overall system performance of the series system and the parallel system are compared from three aspects of thermodynamics, economy, and exergoenvironment to evaluate the basic performance of the two systems under initial conditions. Next, the performance variations of both systems are assessed by varying the compressor outlet pressure, flash pressure, R14 mass flow rate, and heat source temperature. Finally, the Multi-Objective Cuckoo Search algorithm is used to optimize the systems for two and three objectives, taking the exergy efficiency, payback period and product unit exergoenvironmental impact as objective functions. The final results indicate that the three-objective optimized parallel system has the best performance, the exergy efficiency, payback period, and product unit exergoenvironmental impact of that is 62.25%, 1.389 years, and $7.799 \times 10-3$ mpt/kJ, respectively. By comparing the performance differences between the series system and the parallel system, this study provides application ideas for engineering requirements.

- **Keywords:** Cogeneration system; Thermodynamics; Economy; Exergoenvironment; Multi-objective optimization

Hamid Ahchouch, Abdelkarim Chaouiki, Said Ait Talhajt, Lahcen Bammou, M'hammed Belkhaouda, Rachid Salghi, Young Gun Ko. *Inter- and intra-molecular synergism in designing MgO-MCC composite-based coating: An efficient inhibitor for excellent anticorrosion performance*. Pages 1461-1476.

Polymer-based corrosion inhibitors are characterized by high efficiency, low cost, and eco-friendliness; however, their underlying mechanisms and modes of action remain poorly understood, presenting a significant challenge in optimizing their performance and effectiveness in practical applications. In this study, we successfully synthesized and thoroughly characterized a novel nanocomposite, combining magnesium oxide (MgO) nanoparticles with microcrystalline cellulose (MCC), and assessed its potential as a corrosion inhibitor for XC18 steel in an HCl 1.0 mol/L environment. The anticorrosive performance of the MgO-MCC composite for XC18 steel under harsh acidic conditions were investigated via electrochemical impedance spectroscopy (EIS), potentiodynamic polarization (PDP), and surface characterization with a scanning electron microscope (SEM). Morphological analysis suggested the formation of a protective barrier with a fiber-like architecture on the XC18 surface that hindered corrosion. The electrochemical results revealed an increased inhibition performance of MgO-MCC with increasing concentrations reaching a higher efficiency of 87% at 700 ppm. Also, EIS results displayed maximum corrosion resistance achievement in the presence of MgO-MCC-based material (about 147.50 Ω cm2) along with mixed protection mechanism. Advanced theoretical calculations based on density functional theory (DFT) and first-principles density-functional tight-binding (DFTB) were performed to understand the MgO-MCC behavior at metal interface as well as to explore the inter- and intra- molecular interactions involved in the hybrid material formation, complementing the experimental findings. The interfacial mechanism and structure engineering of MgO-MCC composite for functionalizing the surface of metal alloy were also investigated and discussed. MgO-MCC

benefits from essential inter and intra-molecular interactions, leading to a robust adsorption layer. The parallel adsorption configuration and mutual interaction establish a stable hierarchical self-assembly structure and stabilize the Fe—O bonds, thus improving the chemical and physical bonding with XC18 steel surface. The results suggest that the synergistic combination of MgO nanoparticles and polar-rich MCC is a valuable approach for designing novel hybrid materials.

- **Keywords:** MCC-based material; Inter-/intra-molecular interaction; Nanoparticle; Corrosion inhibitor; Adsorption behavior; Density-functional tight-binding

Guangying Li, Jiyun Wang, Mingyan Wang, Yunru Lin, Xiao Yu, Ruowen Zong. *Experimental and numerical study of heavy gas dispersion in presence of obstacle motion*. Pages 1494-1505.

Most of the current research on heavy gas dispersion focuses on how fixed obstacles affect gas spreading. The turbulence caused by the movements of people or traffic will significantly affect heavy gas dispersion. Accordingly, this study presents an investigation of heavy gas dispersion under the influence of moving obstacles, which is based on the dynamic mesh approach using computational fluid dynamics (CFD). A turbulence model suitable for such a condition has been developed, and we have designed a small-scale experiment to verify the model's viability. Consequently, the verified model is further applied to a full-scale scenario for a chemical factory where a chlorine leak triggers an evacuation movement. On the basis of this scenario, we simplify the massive escape crowd to a regular geometric model, and the effects of the speed and size of movable obstacles on gas dispersion have been investigated by means of the RNG k-ε model and the layering updating approach in the dynamic mesh.

- **Keywords:** Heavy gas dispersion; Movable obstacle; CFD; Dynamic mesh