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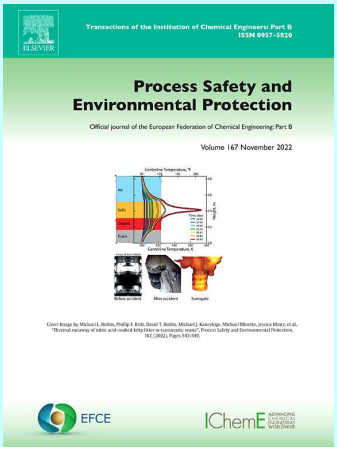

Zhihe Cao, Baozhong Ma, Jiashun Zhou, Yongqiang Chen, Chengyan Wang. *The study for reduction roasting of laterite residue in the presence of CaF2*. Pages 1-9.

Lately, an increasing number of companies invested in the hydrometallurgical process of laterite ores. In the meantime, the research on disposal of laterite residue has come under spotlight the sake of environmental protection, economic efficiency, and resource utilization. Consequently, reduction roasting process in the presence of CaF2 is proposed to treat laterite residue efficiently and recover valuable components. The thermodynamic calculation was conducted to study the mechanism of phase transformation and roasting in the presence of CaF2. It is found that CaF2 would react with iron olivine and chromite to release iron and chromium. In addition, the addition of CaF2 avails the reduction, migration, aggregation, and growth of metallic Fe and Cr. The optimal conditions for addition of CaF2 and temperature is 10% and 1200 °C, respectively. The recovery of chromium reached 95.61% at 10% CaF2 addition from 65.86% without CaF2 addition and the metallization reduction of iron increased from 77.2% to 91.87%. The function of CaF2 was further investigated by the microstructure evolution of roasting products.

- **Keywords:** Laterite residue; Iron; Reduction roasting; Calcium fluoride

Ángela Moratalla, Salvador Cotillas, Engracia Lacasa, Carmen M. Fernández-Marchante, Sonia Ruiz, Ana Valladolid, Pablo Cañizares, Manuel A. Rodrigo, Cristina Sáez. *Occurrence and toxicity impact of pharmaceuticals in hospital effluents: Simulation based on a case of study*. Pages 10-21.

In the University Hospital of Albacete (Spain), the distribution of Active Pharmaceutical Ingredients (APIs) was studied to estimate the occurrence of the most prevalent analgesics and anti-inflammatories and antibiotics in patients' urines. This estimation was based on the consumption amounts of APIs and their pharmacokinetic data. Results showed that metamizole would be the most prevalent drug among analgesics and anti-inflammatories with estimated concentrations ranging 100 – 1000 mg dm−3 in patients'

urines hospitalized in the surgical ICU, followed by around 10 mg dm−3 of acetylcysteine in surgical ICU and paracetamol in geriatrics. Likewise, estimated concentrations of 1–10 mg dm−3 were calculated for the 20 most representative antibiotics. Two β-lactam antibiotics (imipenem, meropenem) and one fluoroquinolone antibiotic (levofloxacin) would be present in patients' urine from more than 3 surgical and medical areas. Additionally, the simulation of the toxicity impacts of active pharmaceutical ingredients (APIs) in hospital effluents was developed using the SimaPro 9.3.0.3 software and Ecoinvent 3.3 database since few studies were reported based on the real occurrence of drugs in urines. Ibuprofen was observed to have 2.4 times more ecotoxicity in freshwaters than paracetamol, although they did not show human toxicity related to carcinogenic effects. Amoxicillin presented a high potential ecological risk with a 3 kg equivalence of 1.4-DB per gram of drug. Overall, results demonstrate the importance to develop an adequate management and treatment of hospital effluents, including hospital urines, to reduce environmental and sanitary impacts.

- **Keywords:** Ecotoxicity; Hospital; Drugs; Wastewater

Yanan Zhao, Zhilu Liu, Mingliang Li, Rui Long, Song Li, Zhichun Liu, Wei Liu. *Screening adsorbent-working solution pairs for adsorption-driven osmotic heat engines based on experimental water adsorption isotherm database and machine learning*. Pages 22-31.

Osmotic heat engines have attracted increasing attention in harvesting ultra-low temperature waste heat. In order to fill the gap in the high-throughput computational screening of adsorbent-aqueous salt solution working pairs for adsorption-driven osmotic heat engines, an experimental water adsorption isotherm database is constructed and eight common salt-water solutions are selected to identify the high-performance work pairs with system energy efficiency as evaluation indicator. The relationship between adsorbent properties, adsorbent structure characteristics and system performance is systematically analyzed. Results revealed that high working capacity and moderate adsorption enthalpy of adsorbents and large osmotic coefficients of salts are beneficial to energy efficiency. Adsorbents with larger accessible surface area, moderate available pore volume and critical pore diameter are favorable. Furthermore, regression machine learning is employed for achieving fast and accurate prediction of the system energy efficiency to accelerate screening. Genetic algorithm is adopted to search for the best-performing working pair properties.

- **Keywords:** Adsorption-driven osmotic heat engine; High-throughput computational screening; Machine learning; Genetic algorithm; Energy efficiency

Amir Mohammad Ali Tabrizi, Samaneh Kakhki, Sogand Kakhki, Maryam Foroughi, Mohammad Hossein Ahmadi Azqhandi. *Azithromycin resistance genes in Escherichia coli isolated from wastewater: Characterization and modeling-based evaluation of factors affecting the prevalence*. Pages 32-41.

Azithromycin is becoming an effective alternative medicine against antibiotic resistant Escherichia coli (E. coli), and in parallel, is frequently detecting in wastewater and fresh water media. The current study aimed to evaluate the presence of azithromycin resistance genes (AzRGs) in E. coli isolated from urban wastewater for which there is a serious lack of information. For this, the samples were collected from four vital points of an urban wastewater treatment plant (WWTP), analyzed for physicochemicfial parameters, and identified for the azithromycin resistant isolates. The isolates were then subjected to 13 other extensively used antibiotics (from seven different classes), including amikacin, aztreonam, ceftazidime, ciprofloxacin, cefepime, ceftriaxone, cefotaxime, doxycycline, gentamicin, imipenem, norfloxacin, tetracycline, and

trimethoprim/sulfamethoxazole; detected for AzRGs, phylogenic group, and molecular typing. The results clearly showed that: a) except for amikacin in all samples and gentamicin in effluent samples, E. coli isolates were resistant to all other the antibiotics studied in the mean respective values of 53.8%, 90.4%, 50%, 40.4%, 86.5%, 86.5%, 63.5%, 13.5%, 73.1%, 46.2%, 65.4%, 69.2%; b) for 75% of them (i.e. except for amikacin, gentamicin, and trimethoprim/sulfamethoxazole), the antibiotic resistance prevalence in effluent samples were significantly higher than that of sludge (p-value = 0.011), aeration (p-value = 0.023), and even influent (p-value = 0.038) samples, suggesting that WWTP facilities acquiring the resistance gene; c) The high values of multiple antibiotic resistance (MAR) index in almost all of the isolates (0.21–0.91) were categorized them in high-risk group, though the values were not found to be influenced by WWTP. Surprisingly, from 10 AzRGs, only two genes of mph(A) and erm(B) were detected in 100% and 67.3% of the isolates, respectively. The prevalence of erm(B) was significantly influenced by MAR index (p-value = 0.004), which MAR in turn, influenced by physicochemical parameters of wastewater in the relative effectiveness of COD (36%) > EC (29%) > TS (16%) > TDS (9%) > temperature (6%) > pH (4%), as modeled using artificial neural network (ANN) approach (R2 = 0.85 and MSE = 0.006302). The phylogenetic group A (59.6%) and clusters of III and V with 23 and 18 isolates, respectively, were dominant among the isolates which both showed a high correlation with MAR indices and therefore erm(B) prevalence. These results were interesting as highlight the effect of WWTP on acquiring antibiotic resistance and AzRGs prevalence in E. coli. Therefore, defining new strategies for relieving the challenge is of great importance.

- **Keywords:** E. coli; Multiple antibiotic resistance; Artificial neural network; Phylogenic group; Molecular typing

Zonghou Huang, Yue Zhang, Laifeng Song, Qiangling Duan, Jinhua Sun, Wenxin Mei, Qingsong Wang. *Preventing effect of liquid nitrogen on the thermal runaway propagation in 18650 lithium ion battery modules*. Pages 42-53.

Thermal runaway (TR) and its propagation in lithium ion battery (LIB) are major factors of inducing serious fire accidents, and their prevention remains a technical barrier. In this work, a novel strategy with liquid nitrogen (LN) to prevent TR propagation (TRP) was proposed and investigated experimentally. Nozzle diameter screening and blank TRP experiments of module were conducted. To comprehensively understand suppression mechanism, LN cooling strategy was analyzed by changing the mass of LN. Results show that 4 mm diameter nozzle owns the best cooling capacity due to its maximum average cooling rate. TRP of a 2 × 3 module presents three typical stages with different TRP time and heating powers. LN exhibits excellent cooling prevention and delay capacity for different stages of TRP. During LN application, the maximum cooling rate and maximum cooling power for single battery reaches 34.25 ℃/s and 1529.6 W, respectively. The critical suppression temperature, Ttr ,cs was proposed to forecast the suppression effect before LN application, and TRP could be prevented below Ttr ,cs. The internal mechanism of LN preventing TRP was discussed in three typical scenarios. This work owns important guidance for process safety assurance and fire protection design of LIB system.

- **Keywords:** Lithium ion battery safety; Thermal runaway propagation; Liquid nitrogen; Cooling power

Arick Castillo-Landero, Jorge Aburto, Jhuma Sadhukhan, Elias Martinez-Hernandez. *A process modularity approach for chemical process intensification and inherently safer design*. Pages 54-66.

Process intensification through hybrid equipment combining unit operations has the potential for reducing energy demand and improving the safety of a chemical process. Selecting which unit operations to combine into an intensified unit is necessary in developing an intensified process that offers an inherently safer design with reduced energy demand. This paper presents a novel methodology to intensify a chemical process guided by modularity. A process network is decomposed into modules by applying a community detection algorithm to find the process units to be integrated into an intensified "module" to improve the Fire and Explosion Damage Index (FEDI). A case study for the separation of an ethanol-butanol-water mixture illustrates this approach. The results show that the safest design (lowest FEDI) is Alternative 1 which was developed using the approach and correlates with high modularity of 0.607. Energy use is reduced by 25.8% thus also leading to a more energy efficient process compared to the non-intensified design with a lower modularity (0.385). A rather empirically guided design was proposed as Alternative 2 which led to modularity of 0.533, but only 10% energy saving and no improvement in the FEDI. This demonstrates that intensification guided by modularity strengthens integration between the process units while improving both safety and energy efficiency. As such, the approach has a wide potential application to guide the intensification of chemical processes.

- **Keywords:** Process intensification; Modularity; Inherently safer design; Ethanol-butanol-water separation

Ana Isabel Díaz, Adriana Laca, Nelson Lima, Mario Díaz. *Treatment of kraft black liquor using basidiomycete and ascomycete fungi*. Pages 67-76.

The Kraft Black Liquor effluent generated by the pulp and paper industry is a highly alkaline solution with high chemical oxygen demand (COD), phenolic content, toxicity, and low biodegradability. Currently, it is usually concentrated and used as combustible in cogeneration systems. However, the profitability of this management depends on the unstable energy prices. As a possible alternative, in this work, different fungi have been used to treat this polluting wastewater. Tests were carried out at 25 ºC and 150 rpm for 10 days in a batch reactor. Two fungi capable of releasing suitable enzymes have been tested, i.e., Aspergillus uvarum and Phanerochaete chrysosporium. The effluent was treated with and without solids and with and without pH control. In all cases, the evolution of COD, biological oxygen demand (BOD5), colour index, and the concentration of reducing sugars and phenolic compounds were analysed. Besides, the enzymatic activities manganese peroxidase (MnP), lignin peroxidase (LiP), and laccase (Lac) were measured. Results showed that the presence or absence of solid did not affect the biodegradation process, achieving similar efficiencies. Bioremediation with P. chrysosporium allowed to obtain removals of COD, colour and phenolic compounds of 65 %, 37 % and 56 %, respectively, while A. uvarum achieved 61 %, 81 % and 67 %, for the best conditions tested. These results give good perspectives for application of both fungi for problematic industrial wastewaters, such as black liquor. It is especially interesting the good results obtained with A. uvarum, which has not been previously tested for the treatment of effluents from the paper industry.

- **Keywords:** Kraft black liquor; Phanerochaete chrysosporium; Aspergillus uvarum; Biological treatment; Phenolics removal; Fungal enzymes

Selvarasu Maheshwaran, Ramachandran Balaji, Shen-Ming Chen, Elayappan Tamilalagan, Narendhar Chandrasekar, Selvarajan Ethiraj, Melvin S. Samuel. *Construction of graphene oxide wrapped gadolinium vanadate nanocomposites as an efficient electrocatalyst for the amperometric sensing of sulfadiazine*. Pages 77-87.

Ultrasensitive detection of antibiotic molecules is fast becoming a vital field of research in recent years. In this research article, we hydrothermally developed a pellet-shaped nanomaterial based on rare-earth metal vanadate (GdVO4) and they are made of composites with graphene oxide (GO). The surface morphology studies through microscopes confirm the effective formation of pellet and sheet-like architectures of GdVO4 and GO. The synthesized nanocomposites are probed for the electrochemical detection of antibiotic sulfadiazine (SLZ). The electrochemical detection performance is investigated through cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and i-t amperometry analysis. The primary composite of GdVO4 @GO displayed superior selectivity and sensitivity to GdVO4 and GO. Through i-t amperometry analysis, enhanced sensitivity of 1.3009 μA μM−1 cm−2 and a limit of detection of 3.1 nM for SLZ detection are achieved. In order to validate the fabricated SLZ sensor, we tested them in real-world biological and environmental samples like human blood serum, river and waste water samples. The GdVO4 @GO-based sensor performed remarkably well with good selectivity for SLZ.

- **Keywords:** Rare-earth metal vanadate; Graphene Oxide; Sulfadiazine; electrochemical sensor; biological and environmental analysis

Jinlong Zhao, Guangheng Song, Xiang Zhang, Yuntao Li, Jianping Zhang, Rui Yang. *Experimental investigation and modeling of the spread and burning behaviors of continuous spill fires on a water surface*. Pages 88-95.

Spill fires caused by oil leakage from tankers may pose a threat to the liquid transportation safety. In this paper, a series of large-scale gasoline continuous spill fire experiments were conducted on a water surface. The spread area, flame height, burning rate and the temperatures in the water layer were measured for different fuel discharge rates and ignition delays. The findings showed that the spread process can be well predicted by an existing spread model without ignition. For ignited conditions, four burning phases were identified, namely (i) spread burning phase, (ii) shrinking burning phase, (iii) quasi-steady burning phase, and (iv) extinguishment phase. The burning rate at the quasi-steady phase was found to be approximately 45–62 % that of pool fires with the same burning area. Subsequently, a model was developed for predicting the quasi-steady burning rate of spill fires. The flame height at the quasi-steady burning phase was also analyzed and correlated with the fuel discharge rate. Finally, a model was proposed to predict the maximum burning area at the spread burning phase and validated against the experimental data. The present results are of practical importance in understanding the spread and burning characteristics of continuous spill fires and the associated risk assessment.

- **Keywords:** Continuous spill fire; Fuel spread; Burning rate; Maximum burning area; Spread model

Wei Huang, Xiaowei Chen, Yi Qin. *A simulation method for the dynamic evolution of domino accidents in chemical industrial parks*. Pages 96-113.

Based on the typical physical effects of different accidents and considering the interaction of time and space, a dynamic evolution model of the domino effect was proposed in this

study. The Monte Carlo method was used to deal with the uncertainty of the evolution path and capture the characteristics of the time evolution. The model considered mixed accident types and the synergistic effect of accidents and extended the application of the probit model. Risk assessment parameters such as evolution path, evolution time, tank accident probability, and domino evolution probability were obtained to evaluate the vulnerability of storage tanks exposed to such hazards. The proposed model was verified through a comparative case analysis, and the results showed that the model can not only capture the space–time dimension but also overcome the limitations of conventional analysis of high-level domino propagation. Different accident types, synergistic effects, and burning capacity of storage tanks have a significant impact on the domino propagation process.

- **Keywords:** Domino effect; Dynamic risk assessment; Monte Carlo method; Spatial-temporal evolution

Yu-Chi Cheng, Shun-Chieh Chang, Chi-Min Shu. *Effects of volatile organic compounds on the explosion characteristics of polyethylene dust*. Pages 114-122.

This study investigated the effects of different concentrations of ethylene and propene gas on the explosion characteristics of polyethylene (PE) dust. After the addition of ethylene and propene gases, the maximum explosion pressure of PE dust increased from 6.7 barg to 9.1 and 7.6 barg by 1.4 and 1.1 times, respectively. Furthermore, the lower explosion limit (LEL) decreased; the addition of even a small amount of these inflammable gases was sufficient to produce a hazardous gas/dust hybrid mixture with low LEL. PE dust tests in a 2 vol. % propene environment revealed that an initial explosion occurred in the hybrid gas mixture, and the heat was transferred to the remainder of the incompletely mixed gas/dust mixture, thereby leading to a two-stage and more complete reaction. In addition, 2 vol. % propene tests also exhibited changes in the maximum pressure rise rate increase, resulting in strong St-2 level explosions because the propene reached its LEL of 2 vol. %. Therefore, propene underwent a complete combustion, resulting in a higher rate of pressure, and shortened time to maximum rate of pressure rise (TMRPR). Thus, the use of volatile organic compounds in dust manufacturing processes considerably increases the risk of explosion incidents.

- **Keywords:** Ethylene; Propene; Lower explosion limit; Inflammable gas; Hybrid mixture

Biao Zeng, Guo Lin, Jing Li, Wei Wang, Libo Zhang. *Selective removal of mercury ions by functionalized Ti-Zr bimetallic coordination polymers*. Pages 123-132.

In order to effectively treat mercury pollution, a bimetallic coordination polymer (Ti/Zr-TA) was successfully synthesized by doping Ti metal for mercury removal in wastewater. The optimum pH (5.0), maximum adsorption capacity (298–318 K: 583.5, 615.4 and 654.4 mg/g), and thermodynamic behavior (endothermic) of Ti/Zr-TA was obtained by batch experiments. The adsorption process conforms to pseudo-second-order kinetic model and Hill isotherm model. Selectivity experiments confirmed that Ti/Zr-TA had a strong interaction with Hg(Ⅱ), which was more easily adsorbed than interfering ions. Adsorption-desorption experiments indicated that Ti/Zr-TA had excellent reusability, and the removal rate decreased by only 15.2 % after four cycles. In addition, the adsorption mechanism was revealed, mercury ions were adsorbated by electrostatic interaction and chelation, in which the chelation between the functional groups containing O, S and Hg(Ⅱ) was dominant.

- **Keywords:** Coordination polymers; Adsorption; Hg(Ⅱ); Selectivity; Mechanism

Eszter Mária Kovács, Dóra Buzetzky, Márton Soha, Tamás Fodor, Péter Kónya, Sándor Stichleutner, Shiro Kubuki, Ernő Kuzmann, József Kónya, Noémi M. Nagy. *Preparation and structure analyses of Sn-bentonite for pertechnetate removal*. Pages 133-141.

Tin (Sn) -bentonite was prepared by ion exchange method from Ca-bentonite. For the ion exchange process, tin-chloride (SnCl2) solution was prepared from metallic tin, and the tin concentration was determined by Microwave Plasma Atomic Emission Spectroscopy (MP-AES). Sn-bentonite was characterized by X-ray fluorescence spectrometry (XRF), X-ray powder diffraction (XRPD), X-ray photoelectron spectroscopy (XPS) and 119Sn as well as iron-57 (57Fe) Mössbauer spectroscopy. 119Sn Mössbauer spectroscopy and XPS undoubtedly revealed both Sn+2 and Sn+4 ions in Sn-bentonite. SnII was attributed to be incorporated into the interlayer space while SnIV located partly in the octahedral position and in the interlayer space of montmorillonite. The removal of radioactive pertechnetate anion (99mTcO4-) was studied on Sn-bentonite in aqueous and artificial urine media. Based on the measurement results, 99mTcO4- ion can be removed, in case of aqueous media, the equilibrium is reached after 5 mins ($x = 99.9 \pm 0.01\%$, $k = 4.2 \pm 0.83$ 1/min) (Buzetzky et al., 2019), while in the case of urine media the equilibrium is reached after 30 mins ($x = 59.1\% \pm 2.7$, $k = 0.18 \pm 0.05$ 1/min). Pertechnetate anoin sorption on tin-bentonite is a (Sn(II/IV)-TcO4-) redox reaction. Thus, Sn-bentonite can be a suitable sorbent for radioactive waste management.

- **Keywords:** Montmorillonite; Sn incorporation; Structural changes; Pertechnetate removal; Radioactive waste management

Fu-Rong Xiu, Chuanzhong Chen, Zhiqi Song, Siyi Wang, Yingying Qi. *A novel resource conversion strategy of waste plastic express packaging bags using supercritical water-ammonia process: Optimization by response surface methodology*. Pages 142-149.

With the rapid development of e-commerce and express delivery industries, a large number of waste plastic express packaging bags (WPEPBs) are generated and urgent to be safely disposed. In this work, a novel resource conversion strategy was developed to produce high value-added chemicals from WPEPBs by supercritical water ammonia (SWA) process without any catalyst. WPEPBs could be converted into two parts by the SWA process: oil and solid residue. More than 80 % of the oil was identified as long-chain alkanes and alkenes due to the decomposition of polyethylene (PE) contained in WPEPBs. The presence of NH3 in SWA was beneficial to improve the production of long-chain alkenes. The plasticizers in WPEPBs including bisphenol A (BPA) and phthalate ester (DEHP) could be efficiently converted into aniline (≈15%) and 2-ethylhexanol (≈4 %) due to the high reactivity of NH3 in the SWA process. Compared with the degradation of WPEPBs in supercritical water, the SWA process could reduce side effects and improve the purity of target products. High-purity CaCO3 powder could be further recovered from the solid residue. The optimal parameters of the SWA process for the conversion of WPEPBs by Response Surface Methodology (RSM) were 440.5 ℃, 90 min, and CNH3 of 4.8 wt%. The conversion ratio of WPEPBs (CWPEPBs) and CaCO3 recovery ratio (RCaCO3) were 99.10 % and 98.85 %, respectively. In contrast to traditional methods for recycling of plastic waste such as mechanical recycling and incineration, the SWA process is believed to be a clean and high-efficiency resource conversion strategy for WPEPBs.

- **Keywords:** Waste plastic express packaging bags; Supercritical water ammonia process; Resource conversion; Response surface methodology

Yan Zhang, Ming Li, Biao Wang, Jiacong Yuan, Ruipeng Tong. *Developing a taxonomy and a dependency assessment model of performance influencing factors for intelligent coal mines*. Pages 150-165.

The arrival of the intelligence era has made the construction of intelligent coal mines (ICMs) a development trend in the field of coal mines, which has caused new human errors in coal mining operations. Therefore, it is necessary to carry out new human reliability analysis (HRA) in ICM operations. The taxonomy and dependency assessment of performance influencing factors (PIFs) can support this necessity. However, the existing taxonomy and dependency assessment model of PIFs cannot effectively adapt to the ICM operation situation. Therefore, based on the current ICM working face system and its operation process, an ICM-PIF taxonomy is developed through a triangulation method and a sociotechnical approach, and a fuzzy Bayesian network (FBN) model assessing PIF dependency is constructed combining the methods of the interpretation structural modeling (ISM), Bayesian network (BN) and fuzzy theory in this study. The results demonstrate that the ICM-PIF taxonomy, including 8 groups and 29 PIFs, is displayed in the form of a visual factor map, and the complex causal dependencies among PIFs are explained through the FBN model from both qualitative and quantitative aspects. The findings provide a traceable and consistent scientific basis for the human error analysis, human behavior modeling and human performance management of ICM working face systems, which could then provide a basic guarantee for the work safety and sustainable development of ICMs.

- **Keywords:** Intelligent coal mine; Performance influencing factors; Taxonomy; Dependency; Fuzzy Bayesian network; Human reliability analysis

Jiaxing Zhu, Lin Hao, WenShuai Bai, Zhenxing Zhu, Bo Zhang, Hongyuan Wei. *A design framework for optimized economic and inherently safe operation conditions for isoperibolic semi-batch reactors*. Pages 166-179.

Thermal runaway in the semi-batch reactors (SBRs) involving exothermic reaction can have serious consequences and the primary driver of process design in the SBRs is economic performance. Hence, in this article, a general framework for safe-economic design and operation of isoperibolic SBRs via integrating advanced process optimization and inherently safe operation condition identification criteria is proposed, and is applied to homogeneous solution polymerization. First, a criterion is proposed to identify the thermally safe operation condition (QFS region, quick onset, fair conversion, and smooth temperature) of homogeneous solution polymerization and the comparison with the other common criteria is conducted. The adiabatic temperature diagrams are also extended to homogeneous solution polymerization considering avoiding triggering side or decomposition reactions under cooling failure. Furthermore, a large accumulation can occur due to the rapid decomposition of the initiator when the jacket temperature in the QFS region exceed a threshold value. Therefore, a new temperature diagram is introduced via combination initiator decomposition temperature and adiabatic temperature diagrams. Finally, the optimal safety-economic design of the simulation case is conducted. The process optimization algorithm is genetic algorithm and runaway criteria are the proposed criterion in this article and the target temperature criterion. The comparison between the target criterion and proposed criterion shows there are almost approximately identical conversion profiles and temperature profiles. This result proves the general proposed framework and further proves the validity of the proposed criterion. This general framework can be extended to other kinetic schemes and this work can contribute to the inherent safety design of semi-batch reactors.

- **Keywords:** Semi-batch reactor; Safe operation; Thermal runaway; Process optimization; Boundary diagram; Safe-economic design

Tran Trung Kien, Nguyen Thi Phuong Thao, Tran Van Thanh, Tran Thi Hieu, Le Thanh Son, Hans Schnitzer, Tran Le Luu, Le Thanh Hai. *Nitrogen conversion efficiency in the integrated catfish farming system toward closed ecosystem in Mekong delta, Vietnam*. Pages 180-188.

In this study, the nitrogen conversion efficiency in the integrated catfish farming system was estimated based on the sludge and wastewater treatment processes. The nitrogen sources were recovered using the composting process (organic fertilizer). The wastewater treatment process was recovered using the aquatic plant uptake (water hyacinths). The sludge waste was mixed with cow dung and water hyacinth biomass at a ratio of 8:1:1. The compost improved the nutrient content of the poor soil, as well as providing additional nitrogen for the plant and limiting the loss of nitrogen sources in the environment. The nitrogen dynamics were estimated using the nutrient biomass flow equality method. The results show that nitrogen was successfully recovered through the composting process and via accumulation in the biomass of the water hyacinths. The nitrogen removal efficiency by using water hyacinth reached 60% after 25–30 days; nitrogen recovery efficiency was found to be 66.94%; and total nitrogen concentration in the soil increased by 53.5% after applying organic fertilizer. The system could be used to recover and reuse nitrogen within the integrated catfish farming circle, under the context of circular economy concept.

- **Keywords:** Nitrogen recovery efficiency; Catfish farming; Composting; Aquatic plants; Biomass flow

Ramesh Chandra, G. Anantharaman. *Treating waste by waste: Remediation of methylene blue using core-shell MI@ZIF-11 nanocomposites from waste toner powder*. Pages 189-204.

Due to the rapid industrialization of printing industries, millions of tons of e-wastes are generated and offloaded to landfills/water bodies, which is hazardous for the environment and a healthy ecosystem. Therefore, researchers are focused on recycling e-waste, for instance, magnetic ink (MI)/toner powder from the cartridge. Herein, MI was successfully activated, encapsulated (wt%: 1–5%) within zeolitic imidazole framework-11 (ZIF-11), and subsequently utilized for wastewater treatment. The crystalline nature of activated magnetic ink (MI), ZIF-11, and their composite was ensured by the PXRD pattern, and encapsulation of MI within ZIF-11 was confirmed by TEM analysis. Furthermore, XPS, BET, UV-DRS, and VSM analyses were carried out to validate the proper encapsulation of MI within ZIF-11. The composites were utilized as an efficient photocatalyst for methylene blue (MB) removal under UV–visible irradiation. MI@ZIF-11 (MZ4) was remarkably found to exhibit 100% removal/degradation efficiency toward MB solution (2 ppm) at pH = 10.71 within 90 min. Moreover, the various factors such as dosing amount of MI (1–5 wt%), catalysts amount (10, 15, and 20 mg), pH (3.03, 5.63, and 10.71), and MB dye concentration (2, 4, and 6 ppm) have been investigated. Further, degradation efficiency, recyclability (up to five cycles), degradation mechanism, and kinetics have been discussed in detail.

- **Keywords:** Magnetic ink (Fe3O4 nanoparticle); ZIF-11; Nanocomposite; Photocatalytic degradation; Environmental remediation; Methylene blue (MB)

Żaneta Arciszewska, Sofia Gama, Barbara Leśniewska, Julita Malejko, Edyta Nalewajko-Sieliwoniuk, Elżbieta Zambrzycka-Szelewa, Beata Godlewska-Żyłkiewicz. *The translocation pathways of rare earth elements from the environment to the food chain and their impact on human health*. Pages 205-223.

Rare earth elements (REEs) have been increasingly exploited for crucial new technologies, and their massive use in the past decades has significantly increased their environmental concentrations. In this article, we have tried to answer the question as to whether or not the wide use of REEs, including nanoparticles, in agriculture and medicine may pose a health risk to the population through diet. For this reason, information on their biological role and potential toxicity to living organisms has been summarised. The fate of REEs in the aquatic and terrestrial environment, such as surface water, soil, soil-plant systems and animals, was described. Particular emphasis was placed on their uptake by plants and animals, translocation between species and thus their entrance into the human food chain. For a better understanding of REEs bioavailability and toxicity, their physicochemical properties, such as e.g. solubility, oxidation state, chemical form, and coordination with ligands are discussed. Data on the estimated daily intake and the presence of REEs in the human body were also compiled. In our concluding remarks we identified gaps in knowledge about the impact of REEs on the population through diet and predicted future research needs in this area.

- **Keywords:** Lanthanides; Biological role; Environment; Bioaccumulation; Trophic chain; Human health

Kexi Liao, Jihui Leng, Y. Frank Cheng, Tengjiao He, Guoxi He, Shuai Zhao, Xin Liu, Qiang Huang. *Effect of H2S concentrations on corrosion failure of L245NS steel in CO2-O2-H2S system*. Pages 224-238.

The corrosion behavior of L245NS steel with different gas environments and H2S concentrations in CO2-O2-H2S environment were studied by weight-loss test and surface characterization techniques. It was found that in the CO2-O2-H2S environment, the H2S, CO2, and O2 reacted successively, and the deposition and hydrolysis acidification of elemental sulfur aggravated the occurrence of localized corrosion. When H2S changed in the low concentration range (1000 – 5000 ppmv), the reaction was dominated by the gradual development of the dense inner film, which decreased the corrosion degree. At 10,000 ppmv, the solution pH value would decrease. More H2S was involved in hydrogen evolution corrosion and enhanced the synergistic effect with O2 to accelerate the corrosion.

- **Keywords:** Multi-component thermal fluid; CO2-O2-H2S environment; H2S concentration; L245NS steel; Elemental sulfur

Wang Xin, Yahan Wu, Xiaohan Ma, Aoda Wang, Liya Wang, Xing Li. *Removal of bisphenol A (BPA) by fermented sludge-derived granular biochar from template-like method: From batch experiment to continuous operation*. Pages 239-247.

Endocrine disruptors have biological toxicity and can interfere with the endocrine system of organisms. They widely exist in natural water bodies. Here, the granular biochar was prepared from fermented sludge for the first time by using cationic polyacrylamide as template agent via a template-like method. The as prepared biochar was investigated for the removal of BPA in aqueous media by batch experiment and continuous flow experiment. The pyrolysis temperature and template concentration had a great influence on the properties of residual biochar and BPA capture. The static adsorption results show that when the template concentration was 1% with the pyrolysis temperature of 800 °C,

the optimal biochar P-1%− 800 achieved the BPA adsorption value up to 84.78 mg/g. Its adsorption behavior, influencing factors, and recycling capability on BPA reduction were evaluated. Kinetics, isotherms and characterization analysis suggested that the adsorption mechanism involved pore filling, electrostatic attraction, π-π interactions and hydrogen bonding. Good regeneration performance, low concentration heavy metal leaching and lasting continuous flow stability in fixed-bed device under different water quality background demonstrated that fermented sludge-derived granular biochar P-1%− 800 is a desirable adsorbent for reducing BPA in complex water environment.

- **Keywords:** Bisphenol A; Fermented sludge; Biochar; Template-like method; Fixed bed

Tao Wang, Peng Yang, Weizhai Yi, Zhenmin Luo, Fangming Cheng, Xuhan Ding, Xiaofeng Kang, Zairong Feng, Jun Deng. *Effect of obstacle shape on the deflagration characteristics of premixed LPG-air mixtures in a closed tube*. Pages 248-256.

In the present research, the deflagration behaviors of premixed LPG-air mixtures with volume fractions from 4% to 8% and various obstacles at a block ratio of 0.6 were experimentally investigated in a closed tube with a length-diameter ratio of 20.4. The parameters such as explosion pressure, explosion time, pressure rise rate, and revised deflagration index were obtained. Moreover, the flame propagation behaviors were recorded, and the structural evolution of the flame front and the corresponding flame speed were identified and then analyzed. The obtained results showed that the net square and perforated disc obstacles increase the flame speed the most, and the peak value reaches 256.2 m/s. When the flame front reaches close to the end of the tube, the combined effects of the reflected deflagration wave and the vortex-induced by the turbulence drive the unburned mixture to propagate to the burned zone, resulting in a backward flame. The maximum explosion pressure and the revised gas deflagration index of the LPG-air mixture increased for six kinds of obstacles with different shapes. The time to peak pressure was greatly reduced. The mesh square and perforated disc obstacles enhanced the pressure parameters the most. The obtained results are of significance in providing fundamental data on the explosion of LPG-air mixtures, providing theoretical guidance for the design of LPG-related devices and structures, and being useful to develop the corresponding explosion mitigation technology.

- **Keywords:** LPG-air mixture; Deflagration; Explosion pressure; Flame propagation; Obstacle; Block ratios

G.V. Kuznetsov, R.S. Volkov, A.S. Sviridenko, P.A. Strizhak. *Fast detection of compartment fires under different heating conditions of materials*. Pages 257-274.

The paper presents experimental findings for the characteristics of equipment activation for the detection of pyrolysis and flame combustion under different heating conditions of materials. Class A model fires in the experiments involved a group of typical indoor combustible materials (wood, linoleum, cardboard, paper). Three most common causes of fires were reproduced: careless handling of fire (open flame), unsafe operation of heating equipment and electrical short circuits. To identify the characteristics of pyrolysis and ignition (i.e., stages preceding a fire), an automated system featuring fire (heat, smoke, flame) detectors, contact and non-contact temperature measurement instruments, a gas analysis system (CO, CO2, O2) and video recording equipment was used. Following the experiments, the scope of technical equipment (smoke, heat and flame detectors, gas analytical sensors, video recording systems) for the detection of pyrolysis of combustible materials and flame combustion start was determined. The most efficient combinations of equipment, necessary and sufficient for the identification of

pyrolysis of combustible materials, were established for different fire causes. The values of the efficiency coefficients of fire detectors are calculated. It is shown that their values for different types of detectors can vary in a wide range (0.1–0.9). Recommendations were made on upgrading the existing fire prevention systems in buildings and creating new automated ones, allowing faster identification of an incipient fire, considering the specific character of the fire hazard source: open flame, heating equipment, electrical overload.

- **Keywords:** Compartment fires; Pyrolysis of materials; Ignition; Identification; Fire hazard sources

Jun Ma, Yuanyuan Wang, Hang Xu, Mingmei Ding, Li Gao. *MXene (Ti3T2CX)-reinforced thin-film polyamide nanofiltration membrane for short-chain perfluorinated compounds removal*. Pages 275-284.

Per- and polyfluoroalkyl substances (PFAS) are a class of 'forever chemicals' that have become a global concern owing to their innate chemical stability on humans and water resources. The separation of PFAS from water resources via membrane technologies are facing huge challenge. High permeance and rejection membrane are required for PFAS. To achieve this goal, herein, we propose an MXene-reinforced interfacial polymerization of negatively charged polyamide (PA) membranes for high rejection of short-chain PFAS. The morphologies and chemical properties were systematically investigated for the fabricated membrane. Attributed to the hydrophilic of MXene, the permeance of MXene-PA membranes increased without sacrificing rejection. Density functional theory (DFT) calculations and various experiments elucidated in detail the underlying mechanism of the interactions between the membrane and PFAS. The enhanced electrostatic interaction and hydrogen bonding leaded to increased PFAS rejection and permeance. Therefore, the MXene-regulated PA membrane effectively solved the trade-off between the selectivity and permeability. This work shows that MXene-regulated interfacial polymerization techniques can be used to tailor the effectiveness of PA nanofiltration membranes to overcome the trade-off phenomenon and pave the way for solving the crisis of short-chain PFAS.

- **Keywords:** Nanofiltration; MXene polyamide membrane; Short-chain PFAS removal; DFT calculation

Shinuo Wang, Yinghao Ruan, Haosheng Sun, Ludong Yi, Di Liu, Jun Wang, Zhaohong Zhang, Dawei Fang. *Study on degradation of Basic Violet 1 and heat generation by parallel orifice plate hydrodynamic cavitation*. Pages 285-299.

Hydrodynamic cavitation (HC) technology with double parallel orifice plates can further enhance the degradation effect and heat generation efficiency and play an important role in practical large-scale organic wastewater treatment and energy saving. In this study, based on the optimal hole numbers in single orifice plate, the influences of the hole number and distribution in double parallel orifice plate on Basic Violet 1 (BV-1) degradation and heat generation are studied in detail. Furthermore, the effects of some experimental parameters (inlet pressure, initial concentration, solution temperature and solution volume) on BV-1 degradation and heat generation in 4 + 4 parallel orifice plate HC system are deeply studied. Then, the effect of added H2O2 on the BV-1 degradation and heat generation is also investigated. In addition, the capturing experiments of free radicals (•OH and •O2-) are carried out. Finally, the BV-1 degradation pathway and possible degradation mechanism are proposed by analyzing the data of UV–vis spectrum, LC-MS and total organic carbon (TOC). The final results show that the solution temperature can be raised from 20.05 °C to 57.71 °C under the experimental conditions of 4 + 4 parallel orifice plates, 3.0 bar inlet pressure, 5.0 L total solution volume and

10 mg/L initial concentration for 90 min continuous circulation and the BV-1 degradation ratio can be achieved by 75.98 %. The system can generate 785.40 kJ heat at 48.50 USD/m3 cost and achieve 29.09 % thermal efficiency. For 1:30 molar ratio of BV-1 and H2O2, the solution temperature can be further raised to 63.32 °C in 90 min continuous cycling. 95.38 % BV-1 degradation ratio can be obtained and the 909.72 kJ heat can be generated, reaching the 33.69 % thermal efficiency. It is hoped that this work can provide a new strategy for enhancing the degradation of organic dyes and resource utilization of heat by using double parallel orifice plate HC technology.

- **Keywords:** Hydrodynamic cavitation; Double parallel orifice plate; Degradation of organic pollutants; Heat generation; Thermal efficiency

Chuchai Sronsri, Wanpasuk Sittipol, Napong Panitantum, Kongpop U-yen, Pongsathorn Kerdphol. *An efficient, multi-stage process for recovering gold from electronic waste involving autoclave pre-treatment and industrial-metal pre-extraction*. Pages 303-313.

In recent years, the recovery of gold from electronic waste, especially waste printed circuit boards (PCBs), has grown in importance. PCBs consist of organic epoxy resins overlaid with valuable metals. The first step in recovering metals from waste PCBs is the removal of these resins. In this paper, autoclave-assisted alkaline pretreatment employing NaOH was used to remove resins from the PCBs. The process is shown to remove epoxy efficiently when conducted at 350 °C for 18 h using 0.8 mol·L−1 NaOH, 18 bar, and a liquid-to-solid (L/S) ratio of 18 mL·g−1. After autoclaving, the solid-phase sample (autoclaved powder) was treated with a mixture of FeCl3 and HCl solutions – a process known as "FeH extraction" – to remove industrial metals. Under the optimal conditions (0.8 mol·L−1 FeCl3, 0.6 mol·L−1 HCl, L/S 24 mL·g−1, 50 °C, 100 min, 300 rpm), this process proved highly efficient in removing industrial metals. Following this treatment, a KClO3-HCl-CaCl2 extraction system was employed to extract gold from the FeH-extracted sample. With this system, a 99.5% gold extraction efficiency was achieved under the optimal conditions (0.55 mol·L−1 KClO3, 1.2 mol·L−1 HCl, 1.5 mol·L−1 CaCl2, 60 °C, 80 min, L/S 12 mL·g−1, 350 rpm). Gold ions ($AuCl_4^-$) in the extracted solution were subsequently recovered by using hydroquinone as a reducing agent to form gold nanoparticles (AuNPs) with the assistance of NaOH. Finally, the AuNPs were stabilized using benzoquinone (an oxidized product of hydroquinone).

- **Keywords:** Waste printed circuit board; Autoclave treatment; Epoxy removal; Gold recovery; Hydroquinone; Gold nanoparticles

Xiaodong Xin, Jiaqian Xie, Wei Li, Sihao Lv, Junguo He. *New insights into microbial fuel cells for saline wastewater treatment: Bioelectrogenesis evaluation, microbial interactions and salinity resource reuse*. Pages 314-323.

This first-attempted study displayed the multi-skilling performance of microbial fuel cells (MFCs) for treating saline wastewater in terms of soluble organics biodegradation, bioelectricity conversion, redox-mediators obtainment and salinity reuse. Results indicated that a bioelectricity conversion efficiency of ca. 0.865–0.960 kWh/kg CODMn with over 90% organics removal in 10.0–20.0 g NaCl/L conditions could be realized. Meanwhile, the redox mediators-like substances could be enriched from saline wastewater via MFCs treatment, which exhibited relatively high redox properties as electron shuttles. Moreover, the dominant members of Bacteroides, Azospirillum, Dyella, Sphingomonas, Ignavibacteriales and Clostridium cooperated together for completing bioelectrogenesis effectively with high capabilities of salinity tolerance. Higher salinity (ca. 30.0–40.0 g NaCl/L) impaired key hydrolase activities, reduce microbial metabolic functions and weaken anodic microbial diversity, which negatively reduce MFCs' running

properties. Finally, the harvested salinity from saline wastewater through MFCs could be used effectively as a promising way of achieving waste sludge solubilization. This study could help to re-shape the thinking about future saline wastewater and excess sludge treatment/management toward resource recovery and cost minimization.

- **Keywords:** Microbial fuel cells (MFCs); Saline wastewater; Redox mediators harvest; Microbial metabolic functions; Salinity reuse

Xiaojing Peng, Wei Zeng, Haohao Miao, Sijia Lu, Shuangshuang Li. *A novel carbon adsorbent derived from iron-poisoned waste resin for phosphate removal from wastewater: Performance and mechanism*. Pages 324-335.

In this study, a new Fe-rich carbon composite derived from iron-poisoned waste resin (WRC) was successfully prepared via pyrolysis-activation to remove phosphate from wastewater. The physicochemical properties of WRC were characterized using multiple characterization tools. The results showed that the WRC had a large specific surface area and was rich in metal loading for adsorption. Batch and fixed-bed experiments investigated the adsorption performance of WRC. The maximum adsorption capacity calculated from the Langmuir model was 17.43 mg/g at 298 K. Kinetics experiments showed that the adsorption of phosphate by WRC accorded with pseudo-second-order kinetic model. The WRC could maintain excellent adsorption performance in a wide pH range of 2–12, suitable for various wastewater conditions. Meanwhile, the WRC had well anti-interference of common anions and humic acids on phosphate adsorption and WRC reuse performance. The mechanisms of phosphate adsorption by WRC were confirmed to be electrostatic attraction, ligand exchange and Lewis acid-base interaction. Fixed bed experiments were conducted for dynamic treatment of synthetic wastewater and actual wastewater, and the results indicated that WRC had potential application prospect. This study provides an economically feasible method for the phosphate removal from wastewater and achieves the reuse of waste resin.

- **Keywords:** Phosphate removal; Carbon composite; Adsorption; Synergistic mechanism; Waste resin

Hu Cui, Yang Ou, Lixia Wang, Baixing Yan, Meiwen Bao, Fachun Guan. *Tetracycline hydrochloride-stressed changes in phosphorus fractions during swine manure composting: Emphasize on phosphorus functional genes*. Pages 336-343

Available information on the phosphorus (P) transformation under tetracycline hydrochloride (TCH)-stressed conditions: Emphasize on phosphorus functional genes, during the composting process has received less attention. Thus, this research explored the variation in P-fractions and P functional genes, as well as ascertained the potential microbial phylum carrying P functional genes during the TCH-amended composting. P-fractions was as the following order: Org-P (66.74–69.28%)>Ex-P (14.18–24.96%)>Ca-P (7.29–18.05%)>Al-P ≈ Fe-P ≈ O-P. During the composting process, Ex-P was converted into Ca-P, resulting in a 7.73–10.48% decrease in P-bioavailability. Low-concentration TCH (50 mg/kg) increased the abundance in gcd, pqqc, appA and phoA genes at the temperature- cooling and maturation phases. While TCH reduced the abundance in phosphorus functional genes affiliate to bacteria, but not to fungi. These conclusions can provide basic data for the directional research on the P-dissolving microbial inoculants.

- **Keywords:** Co-composting; Tetracycline hydrochloride; Phosphorus fractions; Phosphorus functional genes

Ali Aldrees, Hamad Hassan Awan, Muhammad Faisal Javed, Abdeliazim Mustafa Mohamed. *Prediction of water quality indexes with ensemble learners: Bagging and boosting*. Pages 344-361.

One of the most crucial jobs to improve water resources management plans is the assessment of river water quality. A water quality index (WQI) takes multiple water quality factors into account simultaneously. Traditionally, derivations of sub-indices for WQI computations take a long time and are frequently rife with errors. The adoption of reliable and effective machine learning (ML) algorithms has become essential for predicting the WQI of such a matrix. This study predicts WQI, i.e., total dissolved solids (TDS) and electrical conductivity (EC), using ML techniques, including individual learners in conjunction with ensemble learners (bagging and boosting). Anaconda (Python) is utilized to accomplish this. Weak ensemble learners are incorporated to create a strong ensemble learner using an adaptive boosting technique, ensemble learner bagging, and random forest (RF) as a modified bagging method. The ensemble learners are employed on weak or individual learners, which include multi-layer perceptron neural networks (MLPNN), support vector machines (SVM), and decision trees (DT) using regression. The data comprises 372 data readings collected on a monthly basis and eight characteristics to forecast the results. Twenty boosting and bagging sub-models were trained on the collected data readings, and they were then optimized to produce the highest R2. Additionally, K-Fold cross-validation with R2, RMSE, and MAE is used to validate the testing data. Furthermore, a statistical model performance index is used to compare ensemble models to individual ones (e.g., MAE, RMSE, NSE, MSE, and RMLSE). The outcome revealed that using the boosting and bagging learners improves the response of individual models. RF, with an R2 of 0.958 and 0.964 (TDS and EC), and DT, with bagging having an R2 of 0.954 and 0.961 (TDS and EC), reported the fewest errors and provided the most reliable and precise performance of the models. In general, the ML ensemble model would improve the performance of models.

- **Keywords:** Total dissolved solids; Electrical conductivity

Jiankai Xie, Peiyuan Chen, Jin Li, Ying Xu, Yi Fang, Aiguo Wang, Jialai Wang. *Directly upcycling copper mining wastewater into a source of mixing water for the preparation of alkali-activated slag materials*. Pages 362-371.

Mining wastewater (MWw) in tailing ponds is one of the major obstacles in reusing tailings in practice and should be disposed preferentially. This paper investigated the feasibility of exploring MWw from copper mining as a source of mixing water to prepare activators for alkali-activated slag materials (AASM). Four MWws with different concentrations were prepared by using MWw to replace all, 1/2, 1/3, and 1/4 of tap water. The influences of different MWws on the setting time, hydration kinetics, hydration products, compressive strength, nano-mechanical properties, pore structure of AASM were investigated. Experimental results confirmed that MWw can be upcycled as the partial or total mixing water for alkali-activated slag materials. The influence of MWw on the properties of AASM was related to its concentration. MWw with low concentrations accelerated the hydration of slag at early ages, nevertheless raw MWw without dilution slightly impeded the hydration process. Although no new hydration product is induced by adding MWw, both NMR pore analysis and nanoindentation testing suggested that the addition of MWw densified the hydration products, which is beneficial for mechanical properties of AASM. As a result, the 28d compressive strengths of AASM increased with increased concentrations of MWw by − 0.8 to 19.9%. Through this paper, a low-cost, green and practical method was developed as an option for the disposal and recycle of MWw.

- **Keywords:** Alkali-activated slag materials; Hydration properties; Copper tailings; Mining wastewater; Nanoindentation

Fatih Yilmaz, Murat Ozturk. *Parametric assessment of a novel renewable energy based integrated plant with thermal energy storage for hydrogen generation and cleaner products*. Pages 372-390.

Renewable energy-supported multigeneration plants and energy storage systems have important in reducing carbon emissions and also effective use of energy sources. In this study, both a renewable energy source-based energy storage process and a newly developed multigeneration plant are studied through detailed thermodynamic analysis. Here, the energy required for the compressed air storage unit is obtained from the hybrid system of solar and wind energy, and the stored compressed air reacts with natural gas in the Brayton cycle and goes to the multigeneration cycle. Furthermore, the key aim of this research is the examination of a multigeneration system for power, heating, cooling, hot water, and hydrogen generation using energy and exergy efficiency methods. The investigated model includes a thermoelectric generator, an organic Rankine cycle, a hydrogen production and liquefaction unit, a cooling system with an ejector, a Brayton cycle, a Rankine cycle with three turbines, and a compressed air energy storage unit with solar photovoltaic and wind turbines. Moreover, to observe the impact of some substantial design variables on the proposed subsystems and the entire plant's performance and irreversibility rate, thermodynamic analysis is applied parametrically. In light of assessment findings, the net power generation rate of the entire system is 31,308 kW at 25 °C reference condition. Also, the net hydrogen generation capacity, cooling capacity, and heating capacity of the total plant are 0.0499 kg/s, 3650 kW, and 4281 kW. In conclusion, the energetic and exergetic efficiencies of the entire model are determined as 0.5258 and 0.4867.

- **Keywords:** Energy; Exergy; Energy storage; Combustion; Hydrogen; Clean multigeneration

Jinliang Zhu, Zhentao Zhang, Zhiming Wang, Guoxiang Li, Shuzhan Bai. *Experimental study on the performance and diagnosis of hydrothermally aged selective catalytic reduction over a copper-based catalyst*. Pages 391-398.

The conversion of nitrogen oxides (NOx) by hydrothermally aged copper (Cu)–based selective catalytic reduction (SCR) is an irreversible phenomenon. Tail exhaust NOx emission control and on-board diagnostics (OBD) monitoring are difficult with hydrothermally aged Cu–based SCR because the on-board NOx sensor has cross sensitivity to NH3 in the exhaust. In this study, the performance and diagnosis of hydrothermally aged SCR under real engine exhaust were studied. The influence of hydrothermally aged SCR on NH3 storage, tail exhaust NOx, urea injection, and OBD diagnosis were quantitatively analyzed under the World Harmonized Transient Cycle (WHTC). The results show that hydrothermally aged SCR had a great influence on the NH3 storage capacity. In terms of SCR conversion efficiency and OBD detection, compared with fresh SCR, hydrothermally aged SCR was more sensitive to space velocity than to temperature. Under different OBD monitored release conditions, the NOx conversion efficiency was greatly different; hence, the occurrence of a false diagnosis can be avoided through the selection of appropriate release conditions. These research results provide a reference for SCR size design, NOx control, and diagnostic strategies.

- **Keywords:** Selective catalytic reduction; Hydrothermally aged; Diesel exhaust; On-board diagnosis

Wei Yu, Chao Liu, Qibin Li, Liyong Xin, Shukun Wang. *Resource utilization of waste HFC-134a refrigerant by supercritical gasification method: A reactive molecular dynamic study*. Pages 399-409.

Effective treatment of HFCs (hydrofluorocarbons) waste refrigerants is of great significance for reducing greenhouse gas emissions. In this study, the supercritical water gasification method was applied to the treatment of waste HFCs refrigerants in order to realize the harmless treatment and resource utilization at the same time. Taking widely used HFC-134a (1,1,1,2-Tetrafluoroethane, CF3CFH2) refrigerant as the research object, the gasification mechanism of HFC-134a in supercritical water was studied by the ReaxFF-MD, and the effect of temperature, reactant concentration and pressure on gasification was studied. The results show that the main products of HFC-134a gasification in supercritical water are HF, H2, CO and CO2. HF is mainly generated by the hydrogen extraction reaction between F radicals and H2O molecules, and the energy barrier is only 31.3 kJ·mol−1. H2 is mainly generated by the hydrogen extraction reaction between H radicals and H2O molecules and H atom-containing molecules or radicals. When the F, H radicals and H2O undergo hydrogen extraction reaction, a large number of OH radicals are generated, and the carbon-containing radicals combine with OH radicals to undergo a reforming reaction. After further removal of H and F atoms, CO and CO2 are ultimately generated. Parametric analyses show that higher reaction temperature can speed up the reaction rate and improve the yields of CO and H2; Lower reactant concentrations help to increase the yields of CO2 and H2 and have little effect on the yields of HF and CO; Higher pressure boosts the reaction rate to increase CO2 and CH4 yields but decrease the yields of HF, CO and H2.

- **Keywords:** Waste refrigerants treatment; HFC-134a; Supercritical water gasification; ReaxFF-MD; Gasification mechanism; Parametric analysis

Shengquan He, Shengnan Ou, Yao Lu, Longzhe Jin, Tuo Chen, Yanran Ma. *Failure mechanism of methane drainage borehole in soft coal seams: Insights from simulation, theoretical analysis and in-borehole imaging*. Pages 410-421.

Methane drainage borehole in soft coal seams is prone to instability. This could seriously compromise methane drainage efficiency, leading to risks of methane hazards at coal mines. In this paper, the failure of methane drainage boreholes in soft coal seams is studied through theoretical analysis, numerical simulation and field monitoring methods, which aims to guide the borehole protection and improve the methane drainage capacity. The functional relationship between effective radial normal stress and effective tangential shear stress at the unstable position of the borehole and the in-situ stress and pore pressure is constructed through the theoretical study. The equation to derive borehole wall collapse pressure is established, considering cohesion, internal friction angle, coal seam porosity, pore pressure, in-situ stress and other factors. The numerical modelling shows that the coal around the borehole undergoes tensile breakage towards the borehole in both single and multiple borehole conditions. The vertical displacement at the borehole top is the largest and the borehole turned into an elliptical shape under compression. Also, it shows the opening and the end of the borehole are at higher failure risks than middle sections. The horizontal and vertical displacements of multiple boreholes are larger than that of a single borehole. While the usage of multiple boreholes improves the methane drainage efficiency, it brings more challenges to the borehole stability. The creep deformation law of borehole is revealed based on new developed in-borehole imaging monitoring system, including four stages: first (transient), second (steady-state), tertiary (accelerating state) and closure. The field measurement shows that the methane drainage efficiency was relatively high in the first two stages, and then the efficiency dropped rapidly when borehole closing. The research results are critical for

guiding methane drainage borehole protection, improving the methane drainage efficiency and enhancing safety in production.

- **Keywords:** Soft coal seam; Borehole collapse; Methane drainage efficiency; Stress distribution; Borehole imaging system

Xiaona Dong, Ruonan Feng, Yuanming Jiang, Tianming Cai, Canlan Jiang. *The impacts of temperature, soil-water ratio, and background multiplied inorganic anions on the degradation of organophosphorus flame retardants in soil by peroxydisulfate-based advanced oxidation processes*. Pages 422-433.

Soil contamination by triphenyl phosphate (TPHP) has posed a potential threat to human health. In this study, the degradation of TPHP by different chemical oxidation methods, including H2O2, persulfate (PS), peroxymonosulfate (PMS), ferrous ions (Fe2+) activated H2O2, Fe2+ activated PS, heat activated PS (heat-PS), and heat activated PMS, was compared. Heat input could promote the activation of PS to generate highly reactive species (HRS) and the aqueous availability of TPHP for more efficient degradation of TPHP in soil than other methods. As reaction temperature rose to melting point of TPHP (50 oC), the degradation rate sharply increased. The activation energy (Ea) of TPHP degradation in soil was caculated to be 115.57 kJ mol-1. The oxidation capacity per unit PS was about 22.0 M-1. Sulfate radicals (SO4•−) and hydroxyl radicals (•OH) were the major HRS for TPHP degradation in heat-PS system. With increasing of soil-water ratio, the inhibitory effect of soil organic matter (SOM) on TPHP degradation was significantly enhanced. The degradation efficiency was highest under weakly acidic conditions (pH ≈ 4.8). Cl− significantly inhibited the degradation of TPHP in heat-PS system, while HCO3− and H2PO4− had little effects on the degradation of TPHP. After reaction, TPHP in soil could be degraded to be less toxic para-hydroxy triphenyl phosphate (p-OH-TPHP), diphenyl phosphate (DPHP), and phosphate ions (PO43−). This study discloses a sustainable strategy for the remediation of OPFRs-contaminated soil by utilizing heat-PS method.

- **Keywords:** Soil remediation; Organophosphorus flame retardants; Heat-activated peroxydisulfate; Soil-water ratio; Degradation mechanism

Leandro O. Conte, Salvador Cotillas, Andrés Sánchez-Yepes, David Lorenzo, Aurora Santos. *LED visible light assisted photochemical oxidation of HCHs in aqueous phases polluted with DNAPL*. Pages 434-442.

This work focuses on removing hexachlorocyclohexanes (HCHs) found in groundwater polluted with dense non-aqueous phase liquids (DNAPLs) by photo-oxidation with hydrogen peroxide or persulfate using LED visible light and ferrioxalate as the catalyst. Single oxidation tests were also performed to evaluate the contribution of LED-vis light on HCHs removal. Results show that it is possible to attain the degradation of HCHs up to 85% in 420 min with persulfate, whereas percentages lower than 40% are obtained when using hydrogen peroxide. Using both oxidants in the presence of ferrioxalate and LED visible light promotes the generation of hydroxyl and sulfate radicals under circumneutral pH values, which are the main responsible species for HCHs removal. Specifically, an oxidant conversion higher than 50% was achieved during the photochemical treatment with both oxidants, whereas conversions below 20% were obtained in the absence of LED visible light irradiation. On the other hand, DNAPL produced as liquid residuum of lindane production contains other chlorinated organic compounds (COCs), which are susceptible to being oxidized by hydroxyl and sulfate radicals, generating competitive oxidation reactions. The final conversion of chlorbenzenes reaches values close to 100% and HCHs are only effectively removed

when persulfate is used as the oxidant. This better performance indicates that the photo-oxidation of DNAPL polluted groundwater with LED-vis light should be carried out with persulfate to ensure the removal of more dangerous COCs. This confirms the excellent ability of sulfate radicals for C-Cl bond breakdown.

- **Keywords:** DNAPL; Lindane; Persulfate; Ferrioxalate; LED Vis-Light

Zhenglun Tian, Qingrui Shang, Xuhai Pan, Ruyue Zhang, Min Hua, Yilin Zhao, Juncheng Jiang. *Experimental study on explosive boiling mechanism of superheated liquid containing ethanol impurities under rapid depressurization*. Pages 443-453.

In this study, a small visualization device was used to research the dynamic evolution of pressure reactions and bubble nucleation in tanks under rapid decompression. The effect of ethanol impurities on the mechanism of superheated boiling of liquids was investigated. The effect of ethanol impurities on the superheated boiling of liquids under different storage conditions is discussed by studying the pressure characteristic parameters. The experimental results show that ethanol impurities can reduce the bubble nucleation radius, leading to a sharp increase in the number of bubbles and more severe boiling during leakage. Besides, there is a saturation concentration which maximizes the promotion of superheated boiling of the liquid. Under the present experimental conditions, the boiling intensity of ethanol impurities saturates at 3.53%, and this saturation concentration decreases slightly with increasing initial leakage pressure. Ethanol impurities also promote boiling of superheated liquids at different initial liquid levels. This study can provide ideas for the investigation, analysis and prevention of related accidents.

- **Keywords:** Boiling liquid expanding vapor explosion (BLEVE); Ethanol impurity; Two-phase flow; Saturated impurity content; Bubble nucleation

Liangning Li, Wenping Li, Qiqing Wang. *Prediction and zoning of the impact of underground coal mining on groundwater resources*. Pages 454-462.

The protection of water resources near coal mines in arid areas is of great significance to regional geological and ecological environment protection and mining area planning. Determining how to reasonably predict the impact of mining on groundwater resources before exploitation is challenging. Adopting a coal mine in Ningxia, China, as a case study, first, a variable weight model (VWM) for evaluating the potential groundwater yield (PGY) of the target aquifer was established considering geological survey data before mining. Then, the traditional empirical equation was improved according to data for a nearby mining area to predict the height of the water-conducting fracture zone (WCFZ). Then, a zoning standard for the impact of mining on groundwater resources was proposed involving five regions: low, low-medium, medium, medium-high and high. Finally, hydrogeological test data and a borehole video camera system (BVCS) were used to verify the PGY and WCFZ height predictions, respectively, and water resource protection measures were proposed according to the zoning results. The research results could provide a reference for sustainable utilization of groundwater resources and rational planning of both groundwater resources and coal resources.

- **Keywords:** Underground coal mining; Groundwater resources; Confined aquifer; Water resource conservation zoning

Jugoslav B. Krstić, Zvonko B. Nježić, Milan D. Kostić, Boško D. Marić, Olivera D. Šimurina, Olivera S. Stamenković, Vlada B. Veljković. *Biodiesel production from rapeseed oil over calcined waste filter cake from sugar beet processing*. Pages 463-473.

A solid catalyst was prepared from waste filter cake (WFC) from a sugar beet processing plant and used, after calcination at 900 °C within 2 h, for biodiesel production from rapeseed oil and methanol. The calcined WFC (CFC) catalyst was characterized by XRF, FTIR, XRD, TGA/DTG, TPDe, TPD-CO2, SEM, N2 physisorption, and Hg porosimetry. The CFC is a CaO-based catalyst with a rigid, sustainable macroporous structure with the largest particles of 2.0 × 0.5 μm, a specific surface area of 7.3 m2/g, and a basicity of 0.27 mmol/g. It provides high conversion of 97.9% in 1 h at the methanol-to-oil molar ratio of 9:1, the temperature of 60 °C, and the catalyst loading of 10% of the oil mass. Its catalytic efficiency is comparable to the WFC-based nanocatalysts and CaO-based catalysts from natural sources. CFC was reused twice with a negligible decrease in catalytic activity, ensuring a FAME content above 97% in 1 h. The biodiesel produced from rapeseed oil over the CFC catalyst has good fuel properties that fulfill most of EN 14214. Therefore, WFC is a promising source of a low-cost, highly active, basic, and environmentally friendly CFC catalyst, which could reduce biodiesel production costs. From this point of view, this catalyst has great potential for developing the process at the commercial level.

- **Keywords:** Biodiesel; Calcined filter cake; Rapeseed oil; Reusability; Sugar beet; Waste filter cake

Jintao Xu, Xiangfeng Chen, Haipeng Jiang, Wei Gao. *Vented hydrogen-air explosions at elevated static activation pressures*. Pages 474-486.

The flame behaviors and pressure characteristics of vented hydrogen-air explosions at elevated static activation pressures (Pstat) were investigated using a 20 L spherical vessel. For vented flame, it was found that the maximum flame lengths and widths raised with the increase in venting diameters (Dv) and equivalent ratios (Φ) by dominating the concentration of vented unburned gas, while they were insensitive to the change of Pstat. Based on the variation law, non-dimensional formulas for predicting maximum flame length and width were established and the relative error was within 50 %. For internal pressure, the pressure curves were characterized with notably oscillations and an empirical formula coupled with NFPA 68 was proposed with a relative error within 25 %. For external pressure, the mechanism of the external explosion was revealed with the assistance of BOS images. The intensity of external explosion mainly depended on the external flow field intensity and the concentration of the unburned gas. The peaks of external explosion pressure and the pressure recession indices reached their maximum at Dv = 125 mm due to the conflicting effect of the increased Dv.

- **Keywords:** Vented hydrogen-air explosion; Elevated static activation pressure; Vented flame; External explosion

Yan Shao, Han Wu, Wenshan Huang, Qijie Jin, Longji Wu, Xueying Zhang, Haitao Xu. Co-doped carbon nitride nanosheets supported on SMFs for peroxymonosulfate activation to degrade tetracycline. Pages 487-498.

For the treatment of antibiotics contained wastewater, developing a highly efficient catalyst is key to peroxymonosulfate (PMS) activation and antibiotics degradation. In this work, nitrogen-doped carbon nanosheets (NCS) coated sintered metal fibers (SMFs) catalyst was designed and developed, which could positively promote the contacting efficiency between PMS, TC and catalysts. In specific, by the dip-coating of SMFs in the

cobalt-contained dicyandiamide formaldehyde resin and the following pyrolyzing coordinated polymer procedure, it was possible to create a Co-doped NCS catalyst supported on SMFs. NCS with abundant exposed surface active sites could result in a relatively higher catalytic activity. Microscopy studies confirmed the presence of stacked NCS with high Co active sites loading, which was anchored on the surface of SMFs. The developed Co NCS/SMFs catalyst exhibited a highly degradation efficiency of 96% in 240 min. Effects of operating parameters (including PMS concentration and solution pH) on the TC elimination efficicency were also investigated. Additionally, Co NCS/SMFs exhibited good PMS activation activity in the wide pH range of 2.0–9.0, and acceptable recyclability with over 86% TC removal efficiency after five cycles test. According to SEM, XRD and XPS results, highly exposed active metal sites, O defects, Co-Nx sites and reactivity of Co0 in Co NCS/SMFs played an important role in the enhancement of degradation efficiency. Finally, radical inhibition experiment and corresponding EPR test revealedthe presence of $SO_4^{\cdot-}$, ·OH, $O_2^{\cdot-}$ and $^1O_2$ in the TC degradation system, in which singlet oxygen ($^1O_2$) was demonstrated to be the dominating reactive species for PMS activation and TC degradation. This work provided an efficient strategy for developing robust monolithic lamellar catalyst for the continuous PMS activated degradation of TC.

- **Keywords:** Nitrogen-doped carbon nanosheets; Peroxymonosulfate (PMS) activation; Degradation; Tetracycline; SMFs

Valentine Chikaodili Anadebe, Vitalis Ikenna Chukwuike, Sethupathy Ramanathan, Rakesh Chandra Barik. *Cerium-based metal organic framework (Ce-MOF) as corrosion inhibitor for API 5L X65 steel in CO2-saturated brine solution: XPS, DFT/MD-simulation, and machine learning model prediction*. Pages 499-512.

In this study, we report the synergistic effect of a metal ion/cluster (cerium nitrate hexahydrate) with an organic linker (2 methyl imidazole) as a nano-hybrid corrosion inhibitor for X65 steel in CO2 solution. To achieve this fit, a wide empirical study from wet chemical synthesis of Ce-MOF (cerium-metal organic framework), electrochemical method and surface analysis were considered. The empirical data obtained from the electrochemical studies were statistically analyzed via a machine learning model (adaptive neuro fuzzy inference system-ANFIS) considering multi input and single output function (MISO). The outcome revealed that Ce-MOF hindered the dissolution of ferrite and cementite phase of the steel in CO2 solution. The electrochemical impedance spectroscopy (EIS) revealed a significant rise in resistance to charge transfer with an increase in concentration of Ce-MOF. Polarization data indicated that Ce-MOF exhibited mixed-type inhibitor characteristics. The range of inhibition efficiencies were in the range of 97% and 95% at 0.15 wt% Ce-MOF for polarization and impedance studies, respectively. The theoretical study shows a flat adsorption orientation of Ce-MOF on the steel surface. Furthermore, the predictive capability of ANFIS model based on statistical norms; shows that the coefficient of determination (R2) is unity. From the statistical view point, much credibility was attributed to ANFIS model with robust description of the nonlinear interactions between the independent and dependent variables.

- **Keywords:** CO2 corrosion; X65 steel; Nano-hybrid; FE-SEM; Modeling; ANFIS

Jiyun Wang, Xiao Chen, Yuanzhou Li, Mingyan Wang, Xiaoyang Yu, Ruowen Zong, Shouxiang Lu. *Effects of filling level and tray size on the burning behavior of a tank during burning of leaking contents: An integrated experimental and numerical approach*. Pages 513-525.

The prediction of the fire hazard of a tank during burning of leaking contents is significant during the emergency response to tank fire accidents. A detailed investigation was

conducted in small-scale tank fire experiments with different filling levels and tray sizes. The liquid (n-heptane) leaked from the tank and burned in the containment structure (the tray) below, heating the tank and emitting radiative heat flux to the surroundings. The temperature of the leaking contents increased as the heating progressed and eventually reached its boiling point. When the leaking contents boiled and burned, the fire hazard was the greatest because the internal pressure increased rapidly, and the mass burning rate and thermal radiation reached a maximum. Modifying the previous models, this paper proposed a virtual tray modeling approach for predicting the mass burning rate and thermal radiation during the burning of boiling leaking contents. The maximum relative error between measurement and prediction was approximately 20%, indicating the availability of the modified models. A three-dimensional transient simulation was set up using the computational fluid dynamics (CFD) technique to predict the temperature response of the leaking contents, and thus, the elapsed time before boiling and burning of the contents was well predicted. These results can provide scientific support for emergency response teams to control similar tank fire accidents.

- **Keywords:** Tank fires; Burning of leaking contents; Experiments; Virtual tray modeling approach; CFD simulation

Jack M. Altwal, Tomasz Olewski, Luc N. Véchot. *Development of a model for the prediction of the ignition properties of combustible dusts undergoing homogeneous combustion: Application to sulfur dust*. Pages 526-534.

The determination of ignition properties such as the minimum explosible concentration (MEC) is critical for the control of the risks associated with handling combustible dust. This work describes a novel approach for the determination of the MEC of combustible dusts undergoing homogeneous combustion, using sulfur dust as a case study. The proposed model is developed based on the heat and mass transfer occurring when a sulfur dust particle in a control volume is exposed to a hot planar surface acting as an ignition source. The model includes radiative and convective heat transfer from the ignition source to the particle and predicts the dust particle's fusion and vaporization. Ignition criteria of sulfur vapor accumulation in the control volume are based on the material's lower flammability limit (LFL) and the comparison of accumulated energy in the control volume to the activation energy of the vapor-air combustion initiation reaction. The model also includes a correlation describing a time to ignition which accounts for necessary dynamic changes like the exposure time of the dust to the ignition source. The model is capable of predicting the influence of the dust particle diameter on the MEC of sulfur dust and was validated with experimental data.

- **Keywords:** MEC; Homogeneous combustion mechanism; Sulfur; LFL

Chunguang Hou, Qiang Guo, Ngie Hing Wong, Jaka Sunarso, Zhixia Li, Xufeng Song, Peng Song, Yuelian Peng. *Preparation of a fouling-resistant Teflon/PVDF composite membrane and its application to treat nanofiltration brine from landfill leachates*. Pages 535-543.

Landfill leachates (LFLs) pose a severe environmental threat given their high strength and the slow degradation nature of their organic and inorganic pollutants constituents. Hence, they are challenging to treat by conventional wastewater treatment methods. Although membrane distillation (MD) is promising for wastewater treatment, membrane wetting and scaling that lead to membrane fouling are the bottlenecks in applying this technology to LFLs. In this work, a commercial Teflon emulsion was used to modify the PVDF membrane via a simple dip-coating method, followed by depositing the PTFE particles onto the membrane surface via thermal curing crosslinking reaction. Hence, a Teflon/PVDF composite membrane was successfully prepared with resistance to sodium

dodecyl sulfate wetting, CaSO4 scaling, and humic acid fouling. Effects of the Teflon emulsion concentration and dipping time on the composite membrane's chemical composition, surface characteristics, porosity, mechanical properties, liquid entry pressure (LEPW), and direct contact membrane distillation (DCMD) performance were systematically investigated. The results showed that Teflon emulsion modification could improve the membrane surface's hydrophobicity, reduce pore size, and increase mechanical strength. The Teflon/PVDF composite membrane with 100% Teflon emulsion and 10 min dipping time exhibited the highest hydrophobicity and 144.3º water contact angle. The M100-10 membrane also exhibited stable performance for treating nanofiltration (NF) brine collected from the LFL. When concentrating the NF brine, the M100-10 membrane achieved only a 7.1% flux decay rate. Hence, the Teflon/PVDF composite membrane demonstrated excellent wetting, scaling, and fouling resistance. This dip-coating method is simple, low cost, easy to scale up, and has potential in the large-scale production of hydrophobic porous membranes.

- **Keywords:** Anti-fouling; Dip-coating; Landfill leachate; Membrane distillation; PVDF membrane; Teflon emulsion

Jingtao Sun, Gongxing Yan, Azher M. Abed, Aman Sharma, R. Gangadevi, Sayed M. Eldin, Mohammad Taghavi. Evaluation and optimization of a new energy cycle based on geothermal wells, liquefied natural gas and solar thermal energy. Pages 544-557.

Today, due to the increase in environmental crises and the challenges facing fossil energies, it seems necessary to exploit and use renewables. Solar and geothermal energies can be integrated as a clean and promising energy production system to produce different forms of useful energy. The existing geothermal wells in Sabalan power plant provide different thermodynamic characteristics. In this regard, this paper develops the thermodynamic-conceptual design and optimization of a new energy cycle based on Sabalan geothermal wells. The considered energy process is based on two flash cycles (FCs), and two bottoming cycles (a Kalina cycle (KC) and a CO2-based Transcritical Rankine cycle (CTRC)). KC and CTRC can increase the level of power generation. Besides that, in the planned energy process, heat exchangers are employed in order to reduce energetic and exergetic losses to transfer thermal energy to a liquefied natural gas cycle (LNGC). LNGC can improve the electrical energy production level. Further, it can supply natural gas (NG) to consumers in the suburbs of the power plant. Additionally, a solar energy system based on parabolic trough solar collectors (PTSCs) has been embedded in order to produce a part of the thermal energy of the energy process. In order to achieve optimal results, the genetic algorithm has been applied to optimize the energetic and exergetic performance of the considered energy process. Based on the research outcomes, the total electricity output of the designed energy process is approximately equal to 26.1 MW. Energy efficiency of almost 24.9% and exergy efficiency of nearly 53.4% are calculated for the energy cycle. Furthermore, the total exergy destroyed through the energy process is approximately 29.5 MW. Under the optimization results, the rates of energy efficiency improvement and exergy destruction reduction for mode A (with NG production) are 17.9% and 3.53%, respectively. Besides, for mode B (without NG production) the rates of energy efficiency reduction and exergy efficiency improvement are 31.7% and 22.1%, respectively. Finally, it was found that, on average, almost 112 collectors are required to supply heat based on the assumption of using solar energy.

- **Keywords:** Geothermal; Single flash cycle; Liquefied natural gas; Solar energy; Energy and exergy analysis; Optimization

Sanad Altarawneh, Mohammad Al-Harahsheh, Chris Dodds, Adam Buttress, Sam Kingman. *Thermodynamic, pyrolytic, and kinetic investigation on the thermal decomposition of polyvinyl chloride in the presence of franklinite*. Pages 558-569.

Thermal co-treatment of Electric Arc Furnace Dust (EAFD) and polyvinyl chloride (PVC) may provide a viable route for reprocessing these hazardous materials within the circular economy. To develop and optimise a commercial treatment process, the complex mechanistic pathway resulting from the reaction of these two wastes must be understood. Franklinite ($ZnFe_2O_4$) is a major zinc containing phase in EAFD and to date, little work has been undertaken on the decomposition of PVC in its presence. Herein, we present a thermodynamic, pyrolytic, and kinetic study of PVC degradation in the presence of $ZnFe_2O_4$. It was found that $ZnFe_2O_4$ decomposed to its associated halides. Additionally, the kinetics data confirmed the catalytic activity of $ZnFe_2O_4$, dropping the de-hydrochlorination onset temperature of PVC from 272 to 235 °C. The distribution of the activation energy with conversion suggests the presence of several competitive reactions each with a different energy barrier. In such a case, reaction channelling can take place leading to selective zinc chlorination. Moreover, since the reduction of Fe_2O_3 is slow at low temperatures, it is recommended to operate at a temperature as low as 235 °C which can promote the chlorination selectivity towards zinc leaving iron bearing compounds in their stable form (Fe_2O_3).

- **Keywords:** Non-isothermal kinetics; Zinc iron oxide; TGA; Activation energy; EAFD; PVC

Mi Yan, Cheng Chen, Li Zhong, Dwi Hantoko, Ekkachai Kanchanatip. *Experimental study on the catalytic supercritical water oxidation of oilfield sludge*. Pages 582-590.

Oilfield sludge is a kind of hazardous waste. In this study, supercritical water oxidation (SCWO) was used to treat oilfield sludge. The effect of operating parameters was investigated, including temperature (390–450 °C), reaction time (5–30 min), oxidation coefficients (OC, 1.0–5.0) and Ni/Al_2O_3 catalyst. The experimental results showed that higher temperature and higher oxidation coefficient favored the degradation of oilfield sludge. Carbon in oilfield sludge was mainly converted to gas phase, for instance, 63.6% of carbon was converted to gas at 5.0 OC, 20 min and 450 °C without catalyst. The removal efficiency of total organic carbon (TRE) could be up to 96.0% at 450 °C, 20 min, and 4.0 OC without catalyst. Furthermore, the addition of Ni-based catalysts could also improve TRE. TRE and carbon conversion efficiency (CE) were 95.2% and 68.2% at 1.5 OC, 20 min and 450 °C with 20Ni/Al catalyst addition, respectively, which were higher than that of without catalyst (89.5% and 33.8%). The characterization and regeneration of catalyst were also carried out. Catalyst Ni/Al_2O_3 had good reliability, the TRE of 92.5% and the catalytic recovery efficiency of 52.6% were observed after three cycles.

- **Keywords:** Oilfield sludge; Supercritical water oxidation; Ni-based catalyst; Catalyst regeneration

Linhu Li, Wen Cao, Pai Peng, Gaoyun Wang, Shi Liu, Hui Jin, Wenwen Wei, Liejin Guo. *Distribution, risk assessment and stabilization of heavy metals in supercritical water gasification of oily sludge*. Pages 591-600.

Supercritical water gasification (SCWG) of oily sludge is a potential handling method for resource utilization and pollution reduction. Heavy metals (HMs) in oily sludge were assessed due to their threat to human health and environmental safety. This work investigated the distribution of four HMs (Cu, Zn, Ni and Cr) under different reaction conditions (550–700 °C, 1–60 min). The concentrations of HMs in liquid residues (LRs)

decreased continuously at higher temperatures and longer residence times except for Ni. Besides, the concentrations of HMs in solid residues (SRs) increased after SCWG except for Zn, and they varied slightly under different conditions. Then, HMs in LRs and SRs were evaluated in terms of Nemerow index, geo-accumulation index and potential ecological risk. The results indicated that the pollution risks of HMs in LRs were minimum at 650 °C and 30 min, while that in SRs changed little. When Na2CO3 was added, pollution risks changed slightly, but nearly complete stabilizations of Cu, Zn and Cr (96.2%, 84.2% and 98.6%) were achieved at 600 °C. Adding Na2CO3 promoted the formation of aluminosilicate to combine with HMs and enhanced their stabilization notably. This work may demonstrate a promising clean way for oily sludge utilization and HMs stabilizing.

- **Keywords:** Heavy metals; Oily sludge; Supercritical water gasification; Stabilization

Juan Pablo Pereira Lima, Elisa Dias Melo, André Aguiar. *Characteristics and ways of treating cosmetic wastewater generated by Brazilian industries: A review*. Pages 601-612.

Raw material diversity and auxiliary inputs for producing cosmetics result in effluents with high polluting potential, usually containing high concentrations of organic low biodegradable compounds, oils and greases, ammonia, surfactants, and salts. Brazil is a country that produces and consumes many cosmetics, and the treated cosmetic industry wastewaters must meet standards established by Brazilian environmental agencies to be discharged into receiving water bodies. This review seeks to evaluate the characteristics of both raw and treated cosmetic wastewaters and the treatment methods adopted by Brazilian cosmetic industries. It was observed a wide variation of COD and BOD5 values for the raw wastewater samples, e.g. COD varied from 850 to 36,000 mg.L−1. More than 50% of the raw wastewaters showed high biodegradability, since BOD5/COD ratio was above 0.37. Conventional treatments have met a minimum 60% removal levels for BOD5, according to current federal legislation. However, few samples fell within the most restrictive state legislation limits, and treatments were not effective in eliminating wastewater toxicity. Interestingly, COD and BOD5 values for raw and treated wastewaters could be linearly correlated (R2 values > 0.8). The straight-line equations obtained in this work can be used to estimate BOD5 from COD data, since the latter is easier to obtain. Regarding alternative treatments evaluated in bench-scale, Fenton processes and electrocoagulation have removed more than 90% of COD in raw cosmetic industry wastewaters. We found reports on reuse practices involving conventionally treated wastewater, which can supply cooling towers at 100% capacity.

- **Keywords:** Industrial effluent treatment, personal care products; Emerging pollutants; Toxicity; Reuse

Hao Feilin, Shen Mingwei. *Ecofriendly removing microplastics from rivers: A novel air flotation approach crafted with positively charged carrier*. Pages 613-623.

Until targeted techniques are developed and implemented, microplastic (MP) particles in freshwater will always exist and remain under consistent growth. In this study, a novel mechanism based on electrostatic -force–-induced aggregation and flotation is proposed to mitigate MP pollution in rivers. First, the air employed as a flotation carrier is first ionized, then. Then, it is dispersed into a circumfluent reactor after the electrons are offset. The four most detected polymers, namely, polyethylene (PE), polystyrene, polyvinyl chloride, and fiber mixture from the cloth washing machine, are pulverized and injected as contaminants into river water and tap water samples to explore the removal characteristics of the configured bench-scale facility. Experimental results suggest that the scheme takes effect rapidly and obtains a maximum removal efficiency (particle

number based) of more than 90% for all four polymer samples in 2 min. The removal behaviors of the MP particles vary with the physical properties of the particles and the operational parameters of the system. The easiest MP particle to separate from the river water matrix is PE. Particles with a diameter of more than 200 μm have high removal efficiency. An in-depth analysis of variance is conducted to determine how the five selected operational parameters affect the system's removal characteristics for the four polymers in the river water sample. Results imply that the proposed process is a promising alternative in tackling the MP problem in rivers because of its short hydraulic retention time, high removal efficiency, no chemical addition requirement, and robustness to polymer types.

- **Keywords:** Microplastic removal; River pollution; Air flotation; Air plasma; Freshwater treatment

Jiaxin Cheng, Hairong You, Minge Tian, Shaoping Kuang, Shuai Liu, Hui Chen, Xuan Li, Huan Liu, Tao Liu. *Occurrence of nitrite-dependent anaerobic methane oxidation bacteria in the continental shelf sediments*. Pages 626-632.

Nitrite-dependent anaerobic methane oxidation (N-damo) is a key bioprocess coupling global carbon and nitrogen cycles and is mediated by NC10 bacteria. So far, the distribution of N-damo bacteria in marine sediments has rarely been reported. In this study, the sediments from the Bohai Sea, Yellow Sea and East China Sea were taken as the research objects, and the ecological distribution of N-damo bacteria was investigated by quantitative PCR and amplicon sequencing. Quantitative PCR results demonstrated that the highest average copy number of N-damo bacterial 16S rRNA gene was in the Bohai Sea, followed by the East China Sea, while the lowest was observed in the Yellow Sea. Based on the OTU numbers, the N-damo bacterial diversity was highest in East China Sea, followed by the Bohai Sea, while lowest in the Yellow Sea. The N-damo bacterial community structure exhibited an obvious spatial distribution among the three seas. Sediment nitrite nitrogen content is the key environmental factor affecting the abundance and diversity of N-damo bacteria, and sediment ammonia nitrogen content is the key environmental factor affecting the community structure of N-damo bacteria.

- **Keywords:** Continental shelf sediment; Nitrite anaerobic methane oxidation bacteria; Ecological distribution; Community structure; Environmental factors

Fei-fei Liu, Tong Lu, Yu-xue Zhang. *Performance assessment of constructed wetland-microbial fuel cell for treatment of mariculture wastewater containing heavy metals*. Pages 633-641.

Mariculture wastewater poses potential risks to the sustainability of the coastal environment. In this study, different types of constructed wetland-microbial fuel cells (CW-MFC), including up-flow CW-MFC (UCW-MFC), down-flow CW-MFC (DCW-MFC), and hybrid up-flow/down-flow CW-MFCs (HCW-MFC) were constructed to evaluate their efficiency to treat mariculture wastewater containing heavy metals (Cu and Zn). The results showed that both the UCW-MFC and DCW-MFC operated with aeration demonstrated better removal performance for conventional pollutants. The presence of heavy metals in wastewater reduced the removal of NH4+-N and total inorganic nitrogen, but had no significant effect on the removal of chemical oxygen demand (COD) and total phosphorus (TP). The HCW-MFC had better removal performance than the UCW-MFC and DCW-MFC, especially when treating heavy metal containing wastewater. All systems had excellent removal performance for (Cu2+ and Zn2+), resulting in concentrations below the first discharge standard. All the systems produced S2-, which could react with Cu2+/Zn2+ to form CuS/ZnS, leading to the removal of heavy metals from the systems. The average output voltage of the three systems was 561.64 ± 16.64 mV for UCW-MFC,

634.73 ± 9.33 mV for DCW-MFC, and 1074.88 ± 49.90 mV for HCW-MFC, respectively. In addition, the maximum power density (PAmax) increased by 160.81 % and 44.16 % in HCW-MFC compared to those of UCW-MFC and DCW-MFC systems, respectively. Further, connecting the three systems successfully derived a light-emitting diode to emit light, which indicated that CW-MFC systems have promising application prospects for both pollutant removal as well as energy recycling.

- **Keywords:** Constructed wetland; Microbial fuel cell; Mariculture wastewater; Copper and zinc

Zhi Wang, Shuya Hou, Muchen Zhang, Jiwei Xu, Zikai Gao, Valerio Cozzani, Bin Zhang. *Assessment of the mass burning rate of LNG pool fires by a validated CFD model*. Pages 642-653.

Liquefied natural gas (LNG) is widely used, because it provides an easy and economic solution to the transport and storage of natural gas (NG), especially on long distances or when transport by pipeline is not viable. The LNG pool fire is one major process safety accident at the LNG facilities according to the report of the U.S. Government Accountability Office. Moreover, due to the high surface emissive power of LNG compared to other hydrocarbon fuels, LNG pool fires have a high potential in causing domino effects and cascading events in process industry. Previous studies developed Computational Fluid Dynamics (CFD) models of LNG pool fires, but the mass burning rate was fixed manually as a model input, not considering that the mass burning rate is determined by the fuel's physical properties and heat input vaporizing the fuel. In this study, a model of LNG pool fire controlled by material physical properties was developed using fire dynamics simulator (FDS), and was validated against LNG pool fire experiments carried out by Mary Kay O'Connor Process Safety Center (MKOPSC). Statistical performance measurement shows that the model is superior to the semi-empirical approaches in predicting the mass burning rate of LNG pool fire under different pool sizes. A flame geometry analysis software was developed comparing different algorithms, and the centroid method was selected. The results show that the fire model (200 kW/m3 as flame contour) can accurately predict the flame geometry observed in the experimental runs. The influence of wind velocity and dike height on the mass burning rate was also investigated. The results show that the height of the concrete dike is negatively correlated with the mass burning rate of LNG pool fire. The effect of wind velocity on LNG mass burning rate is twofold. The forced convective boundary layer at lower wind velocity promotes LNG combustion and increases the mass burning rate, while higher wind velocities reduce the mass burning rate due to the reduction of the thermal radiation feedback. The findings in this study will contribute to an accurate risk assessment of LNG pool fire accidents in the process industry.

- **Keywords:** LNG; Pool fire; FDS; Mass burning rate; Flame geometry; Wind velocity

Chunying Dong, Yuang Pang, Yan Chen, Zhan Gao, Meiqiang Cai, Micong Jin, Zongsu Wei. *Fe-Ti bimetals catalyst derived from biowaste for highly efficient persulfate activation: Performance and mechanisms*. Pages 654-667

Sludge based catalysts (SBCs) has been considered as a promising and viable approach to sludge reclamation. Herein, we fabricated bimetallic Fe-Ti doped SBCs via a facile synthesis with sludge containing polyacrylamide (PAM) as N-precursor. The adsorption capacity and degradation efficiency of as-synthesized SBCs were assessed using tetracycline (TC) as a target pollutant, in which PAM in sludge played a dual role by promoting porosity, active sites, and structural defects beneficial for persulfate (PS) activation. Fe-Ti doping induced the activation of PS by a fast redox cycle of Fe3+/Fe2+

associated with the coexistence of Ti4+/Ti3+, which enabled an efficient electron transfer between the catalyst and PS. The synergistic effect of PAM-derived N doping and Fe-Ti bimetals resulted in prevention of iron leaching and enhanced catalyst stability over a wide pH range. The surface SO4•− was the primary oxidant in the TC degradation process based on free-radical quenching experiments, and degradation pathways of TC were proposed given the intermediate evidence from UPLC-HRMS analysis. This study promotes the reclamation of PAM-containing sludge providing an eco-friendly and efficient process to activate PS for wastewater treatments.

- **Keywords:** Sludge-based catalyst; Persulfate; Fe-Ti bimetallic; Redox cycle; Tetracycline; Polyacrylamide

Niloufar Mohseni, Mohammad Haghighi, Maryam Shabani. *Bimetallic Co2+Cr3+LDH anchored AgCl as excellent solar-light-responsive Ag-decorated type II nano-heterojunction for photodegradation of various dyes*. Pages 668-688.

The widespread use of organic dyes in industrial applications consistently endangers the eco-system health. The photocatalytic degradation of organic wastewater has been recognized as a highly promising strategy for combating this environmental issue. Herein, A series of bimetallic Co2+Cr3+LDH anchored AgCl as excellent solar-light-responsive Ag-decorated staggered nano-heterojunctions were constructed using a facile sono-precipitation method and their performance toward degradation of various azo dyes were investigated. Ag-AgCl-CoCrLDH(3:1)-PU exhibited excellent photocatalytic activity by degrading acid orange 7, eosin Y, rhodamine B, methylene blue, and methyl orange with respective efficiencies of 100.0 %, 98.4 %, 94.0 %, 88.7 %, and 86.2 %. The photocatalyst characteristics were determined using XRD, FESEM, TEM, EDX, BET-BJH, FTIR, and UV–vis DRS techniques. The DRS analysis of Ag-AgCl-CoCrLDH(3:1)-PU photocatalyst (Eg = 2.37 eV) revealed that the introducing of LDH in the heterostructure, along with the SPR effect of Ag particles, increased the visible light absorption capacity. Furthermore, the staggered band gap accelerated charge carrier transformation, resulting in a lower recombination rate. Based on the BET-BJH results, integration of LDH combined with ultrasound irradiation increased the SBET and pore volume (Vp) to 19.5 m2/g and 0.052 cm3/g, respectively (compared to bare Ag-AgCl-PU with SBET and Vp of 3.4 m2/g and 0.004 cm3/g, and non-sonicated Ag-AgCl-CoCrLDH(3:1)-P with SBET and Vp of 16.8 m2/g and 0.016 cm3/g). The FESEM and TEM images clearly displayed the significant influence of sonication on well dispersion and de-agglomeration of nanoparticles. Subsequently, the reusability of nanophotocatalyst was examined, and a possible degradation mechanism was suggested.

- **Keywords:** Bimetallic Co2+Cr3+LDH Anchored Ag-AgCl nanophotocatalyst; Staggered heterojunction; Sonochemical-Design; Surface plasmon resonance; Refractory dyes; Wastewater treatment

Lu Jiang, Maozhong Yin, Yankui Tang, Runlan Dai, Lihong Mo, Weiwei Yang, Yi Liang, Kai Huang. *Microfibers shed from synthetic textiles during laundry: Flow to wastewater treatment plants or release to receiving waters through storm drains?* Pages 689-697.

Microplastic particles (MPs), which have been considered as emerging contaminants, are widely found in water environments. In southern China, many apartment owners place washing machines on their balconies, where the separated drain system usually leads to the storm-water pipes, resulting in releasing MPs directly into the environment. In the present study, we firstly obtained the laundry preference of residents in the study area based on a questionnaire survey and then designed a simulated laundry experiment to determine the MFs shed in the laundry process. The approximate amount of MFs

discharged into the environment under various scenarios was estimated. The results showed that type of washing machine and detergent had a great influence on the MFs shedding. The use of a front-load machine and liquid laundry detergent pods (LDPs) can reduce MFs shed in the laundry process. If the laundry effluent generated by washing machines placed on apartment balconies flows into the municipal pipe network and is treated by wastewater treatment plants (Andrea Menéndez-Manjón), the environmental load of MFs can be reduced. Taking Nanning, the capital city of Guangxi Zhuang Autonomous Region, as a case study, the calculated result shows that the number of MFs discharged into the environment decreased by 93% at the optimized laundry mode. This study provides a reference for the control of MFs and the rational revision of the Architectural Design Guidelines in subtropical cities equipped with the diversion drainage system.

- **Keywords:** Laundry-released microfibers; Wastewater treatment plant; Synthetic textiles; Scenario; Storm drains

Qingwei Song, Lei Ni, Juncheng Jiang, Zhiquan Chen, Gang Fu, Hang Yao, Zhen Cheng. *Process optimization and thermal hazard analysis of the preparation of diphenyl sulfoxide using hydrogen peroxide as oxidant*. Pages 698-711.

In this study, diphenyl sulfoxide was prepared by oxidizing diphenyl sulfide with hydrogen peroxide using phosphotungstic acid as catalyst in semi-batch mode. In order to optimize the synthesis process, a four-factor three-level Box-Behnken design was adopted. The result showed that under the optimal condition, namely catalyst concentration 0.19 mmol/mol, oxygen-sulfur ratio 1.08, reaction temperature 30 ºC, and dosing time 15 min, the yield of diphenyl sulfoxide could reach up to 79.05%. In addition, the thermal behavior of synthesis process was systematically investigated using a reaction calorimeter (EasyMax 102) equipped with a situ FTIR monitoring. The receivable mechanism is that H2O2 is activated by the catalyst and subsequently reacts with diphenyl sulfide to produce oxidized product. H2O2 was relatively stable when PTA was used as catalyst. Thermal risk index was used to assess the thermal hazard of H2O2 & PTA. Furthermore, risk matrix method as well as Stoessel criticality diagram was used to assess the thermal risk of the process and an unacceptable risk was obtained. One of the main hidden dangers was the potential chemical splatter caused by decomposition of H2O2. It should be equipped with a pre-set quench or sufficient emergency discharge to avoid further loss. The results of this work proposed a solid foundation for the safe operation of this process and can be further used for scale-up.

- **Keywords:** Diphenyl sulfide oxidation process Box–Behnken design process optimization thermal risk

Han Zhang, Juncheng Jiang, Miao Fei, Lei Ni, Yao Hang. *Thermal hazard characteristics and essential mechanism study of 1-hydroxybenzotriazole: Thermodynamic study combined DFT simulation*. Pages 713-722.

1-Hydroxybenzotriazole (HOBT) as an important fine chemical has been used as reactants, reagents or catalysts in over 6 million chemical synthesis reactions. The thermal decomposition characteristics of HOBT in non-isothermal, isothermal and adiabatic conditions were investigated through differential scanning calorimetry, thermogravimetric analyzer, and accelerating rate calorimeter. The apparent activation energy, thermal safety parameters, and the decomposition reaction pattern of HOBT pyrolysis were obtained based on adiabatic accelerating calorimeter experimental data. HOBT pyrolysis is a rapid exothermic process with large amounts of gas produced, and HOBT can decompose at a temperature substantially lower than the onset temperature.

The severity and probability of HOBT runaway reaction were assessed. The pyrolysis mechanism paths of HOBT were explored by using TG-MS and TG-FTIR experiments couple with density functional theory calculations. The main decomposition products of HOBT were N2, NO, C2H2, C6H6, CO, HCN, and CO2 gases. This study provides guidance for safe production and application of HOBT, and formulating emergency plans for related hazards.

- **Keywords:** Thermal decomposition characteristics; Accelerating rate calorimeter; Thermal safety; Density functional theory; Pyrolysis mechanism path

Wenshuai Bai, Xingyu Wen, Wei Sun. *Classification and optimization of homogeneous reactions with arbitrary reaction orders performed in isoperibolic semi-batch reactors using θMTSR criterion*. Pages 723-736.

Runaway reactions are very dangerous, and studies on them are indispensable. A lot of criteria have been developed to classify different thermal behaviors. A fine criterion (named as MTSRC) for 2-order homogenous reactions performed in isoperibolic SBRs has also been developed in our previous work. In this paper, firstly MTSRC is amended and renamed as θMTSR criterion. Then θMTSR criterion is further extended to reactions with arbitrary reaction orders. Based on θMTSR criterion, the boundary diagrams (BDs) are reconstructed with a wider scope of model parameters and more data points compared to BDs in previous work, and particularly the influence of reaction orders on BDs is studied. Subsequently adiabatic temperature diagrams (ATDs) with arbitrary reaction orders are innovatively plotted. Finally, the practical applications based on θMTSR criterion, constructed BDs and ATDs are discussed. Classification and optimization procedures for this kind of reaction are proposed, and especially a standalone desktop application program (app) is exploited to let users easily execute these two algorithms. A case study is also shown to verify the developed standalone desktop app.

- **Keywords:** Homogeneous reaction; MTSR; Thermal runaway; SBRs; Safe optimization; App

Wenyan Dai, Jiajia Fan, Qian Zhang, Lingqing Wang. *Ecological risk assessment and sources identification of potentially toxic elements in the surface sediments of Qinghai Lake*. Pages 737-747.

The Qinghai Lake, a quintessential representative of the world's plateau inland lakes, has garnered much scrutiny from scholars for its current status of potentially toxic elements (PTEs) pollution. Hence, this study investigated the concentrations and distribution of seven PTEs i.e., Co, Cr, Cu, Ni, Pb, Zn and V. Furthermore, the potential ecological risk index (RI), self-organizing maps (SOM), correlation analysis and positive matrix factorization (PMF) were used to explore the level of risk and sources of pollution in the study area. The study revealed that: (1) the contents of PTEs in Qinghai Lake sediments were lower than other regions, yet 25.0% of Pb and 19.4% of Zn remained above background values, and the spatial distribution was more heterogeneous; (2) the high ecological risk in the sediment was spread mainly in the downstream of the estuary and the vicinity of tourist sites, where the ecological risk index of Pb was the maximum; (3) correlation and model analysis showed that the seven PTEs were homologous, and besides natural sources, transportation, mixed agricultural cultivation and coal-fired sources were presumed to be the main anthropogenic sources of disturbance. In the midst of rapid economic development, environmental pollution of the Qinghai Lake should be strictly controlled to avoid increased risks.

- **Keywords:** Qinghai Lake; Potentially toxic elements; Distribution characteristics; Ecological risk; Sources identification

Shaohua Mao, Zhen Mao, Bo Li, Wenjie Hao, Shishan Liu, Yangyang Hu, Yuji Fang. *Experimental study on behaviors of flame spread over aviation kerosene under forced airflow*. Pages 768-777.

In realistic industrial scenarios, the leakage of aviation kerosene (RP-5) under forced airflow easily leads to fire spread, which seriously threatens the safety of human life and causes enormous economic losses. Therefore, it is necessary to study the characteristic parameters of flame spread over RP-5 aviation kerosene under forced airflow, such as flame tilt angle (θ), flame height (H), and flame spread rate (V). In this paper, the RP-5 flame spread experiments were carried out by varying the speed (u = 0–6 m/s) and direction (concurrent, opposed, and perpendicular airflows) of the forced airflow. The results show that the flame tilt angle increases as the airflow speed increases and finally tends to be stable, while the flame height decreases monotonically with airflow speed. The special behaviors of flame bifurcation and fire spread rate induced by the critical airflow speed are observed. The phenomenon of "flame bifurcation" will occur due to the influence of differential pressure resistance under high concurrent airflow conditions (u > 1 m/s). When the airflow is relatively small (u ≤ 1 m/s), the mean flame spread rate varies slightly with increasing airflow speed. With further increasing the airflow speed (u > 1 m/s), the mean flame spread rate increases with an increase in the concurrent airflow speed while decreasing as the opposed airflow speed increases. By contrast, the mean flame spread rate remains essentially unchanged under all perpendicular airflows.

- **Keywords:** Forced airflow; Aviation kerosene; Flame tilt angle; Flame height; Flame spread rate

Didi Gai, Xin Cui, Tong Wu, Ji Shi, Peitao Zhao, Jing Zhang, Xu Xia. *A-site disubstituted of La1−xSrxNi0.8Fe0.2O3 perovskite on coal pyrolysis volatiles catalytic cracking: Activity and reaction mechanism*. Pages 748-759.

This work focuses on the result of strontium doping on La1−xSrxNi0.8Fe0.2O3 catalytic cracking of coal tar in the COREX process. The results show that Sr doping significantly affected the catalytic performance of perovskite. O2-Temperature programmed desorption (O2-TPD) and X-ray photoelectron spectroscopy (XPS) results show that La0.8Sr0.2Ni0.8Fe0.2O3 (Sr 0.2) has more active oxygen species and higher oxygen mobility. The performance of Sr-doped catalysts is higher than that of LaNi0.8Fe0.2O3, producing less tar and carbon deposition. Moreover, Sr 0.2 exhibited the highest gas yield of 34.6 mmol/gcoal, H2 yield of 27.5 mmol/gcoal, 100% tar conversion rate, and the lowest carbon deposition of 19.4 mg/(g·h). Tar cracking mechanism was proposed by characterization results. The perovskite could serve as a bridge for oxygen migration and simultaneous oxygen supplementation, thus sustaining catalyst activity and durability. The appropriate amount of Sr doping perovskite is favorable to high catalytic activity and anti-carbon deposition at high temperatures. This work could provide some referential value for the highly-efficient cracking of tar.

- **Keywords:** Perovskite catalyst; Sr doping; Coal tar; Catalyst activity; Carbon deposition

Yuansi Hu, Xinglong Chen, Shiqi Mu, Qibin Li. *Extraction and separation of petroleum pollutants from oil-based drilling cuttings using methanol/n-hexane solvent*. Pages 760-767.

Oil-based drilling cuttings (OBDC) have a high content of petroleum pollutants with strong mutagenic, carcinogenic and teratogenic properties. Solvent extraction can effectively separate petroleum pollutants from OBDC. However, single solvent has preferred solubility for different types of petroleum pollutants in OBDC, resulting in a

lower oil removal efficiency. Therefore, based on the polarity difference between methanol (Me) and n-hexane (He), a method was developed to extract petroleum pollutants from OBDC using Me&He. Compared with methanol or n-hexane alone, the oil removal efficiency of compound Me&He was significantly increased to 94.58 %, and 37, 37 and 77 petroleum pollutants were extracted using Single methanol, Single n-hexane and Compound Me&He, respectively. Methanol extraction preferentially solubilised polar molecules such as alcohols and carboxylic acids, while n-hexane extraction preferentially solubilised alkanes and other nonpolar molecules. Compound Me&He compensated for the low solubility of single solvents for petroleum pollutant extraction from OBDC. Additionally, because methanol and n-hexane are not mutually soluble, it was easy to separate the recycled components. Compared with other common solvent extraction technologies, compound Me&He had advantages including simple operation and high oil removal efficiency. This study provided a theoretical basis and technical reference for the efficient processing and resource recycling of OBDC.

- **Keywords:** Oil-based drilling cuttings; Petroleum pollutants; Solvent extraction; Methanol; N-hexane

Tao Zeng, Guohua Chen, Genserik Reniers, Jinkun Men. *Developing a barrier management framework for dealing with Natech domino effects and increasing chemical cluster resilience*. Pages 778-791.

A domino effect triggered by a natural event (a so-called Natech domino effect) represents a typical high-impact low-probability (HILP) event, which may lead to catastrophic consequences. The presence of safety barriers could have an impact on the effects by impeding propagation patterns and mitigating potential consequences. However, coordinating and maintaining safety measures to establish an effective barrier system against Natech domino effects is complicated. In this paper, the concept of what constitutes a safety barrier and the principles of barrier management are reviewed. Subsequently, the complex phenomenon of Natech domino effects is studied at the individual installation level, while the propagation pattern is explored at the system level. The application of safety barriers is discussed with the aim of coping with potential Natech domino effects. A systematic framework of barrier management is developed to establish and improve the barrier system in the whole cycle (design & construction, operation, accident, recovery & improvement) of a chemical industrial area. The challenges are discussed to highlight future study needs.

- **Keywords:** Barrier management; Process industry; Natech domino effect; Risk; Prevention; Chemical industry

Xiaogang Liao, Lin Zheng, Qi He, Gang Li, Li Zheng, Hongmei Li, Tian Tian. *Fabrication of Ag/TiO2 membrane on Ti substrate with integral structure for catalytic reduction of nitrophenol*. Pages 792-799.

In this work, Ag/TiO2 monolithic membrane catalyst was successfully fabricated on alpha-titanium plate by using a facile two-step method. Firstly, a layer of anatase TiO2 film with nanosheet morphology was formed by the hydrothermal reaction in combination with calcination. After photo-deposition in AgNO3 solution under the ultraviolet irradiation, Ag nanoparticles in metallic state were then deposited on the surface of the as-prepared Ti-based TiO2 film. The catalytic performance of the Ag/TiO2 membrane in the presence of NaBH4 was evaluated by taking p-nitrophenol (4-NP) as a pollutant model. The results indicated that the Ag/TiO2 as a monolithic membrane catalyst exhibited excellent catalytic ability and high stability towards 4-NP degradation. During six consecutive recycling runs, the degradation rates of 4-NP were maintained above 73%, with slight difference. This study shows that the monolithic membrane catalyst Ag/TiO2 is a promising material for the degradation of 4-NP owe to its high activity and easy recovery.

- **Keywords:** Monolithic membrane catalyst; Ag/TiO2; P-nitrophenol; Catalytic reduction

Mohamed Abdelgaied, Abd Elnaby Kabeel, Alaa A. Ezat, Mohamed M. Khairat Dawood, Tamer Nabil. *Performance improvement of the hybrid indirect evaporative type air cooler and HDH desalination system using shell and tube latent heat energy storage tank*. Pages 800-809.

The present work aims to build an innovative hybrid system suitable for remote areas that suffer from freshwater scarcity and the continuous rise in the surrounding environment temperatures as a result of the increasing climatic changes. To achieve this goal, an innovative hybrid system for air conditioning and desalination was designed by incorporating the indirect evaporative type air cooler with a solar-assisted HDH desalination unit. In this innovative hybrid system to achieve the maximum possible production rates of freshwater that can be produced from the HDH unit, the shell and tube latent heat energy storage tank (STLHEST) was incorporated with the innovative hybrid system, in addition to the copper tubes filled with latent storage materials that were installed inside the humidifier, to extend the freshwater production time after sunset. The experimental results showed that the integration of STLHEST, as well as copper tubes filled with the latent storage materials installed inside the humidifier with the proposed innovative hybrid system, represents a very effective option that can produce freshwater with rates up to 241.7 L/day, with an improvement of 14.6% compared to the case without energy storage materials. Also, the average value of the cooling capacity of the air cooler during the test period from 9:00 AM to 9:00 PM reached 941.7 Watts. Moreover, the integration of STLHEST, in addition to the copper tubes filled with the latent storage materials with the innovative hybrid system, will improve the gain output ratio (GOR) from 3.6 to 4.12, with an improvement of 14.4%.

- **Keywords:** Innovative hybrid system; Air coolers; HDH desalination; Solar energy; Shell and tube latent heat energy storage tank; Performance improvement

Lan Hee Kim, Daeho Lee, Jongmin Oh, Sungpyo Kim, Seon-Ha Chae, Dongjoon Youn, Youngjin Kim. *Performance of a novel granular activated carbon and gravity-driven membrane hybrid process: Process development and removal of emerging contaminants*. Pages 810-819.

In this study, a novel granular activated carbon (GAC) gravity-driven membrane (GDM) hybrid system with a ceramic membrane was developed for the production of high quality water. The operational performance in water permeability; removal of organic matter; and contaminants of emerging concern (CECs) including microplastics, larvae, and perfluorinated compounds (i.e., perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid(PFOS)) was evaluated. The experimental results indicate that the GAC-GDM hybrid system can overcome the limitations of the GAC (i.e., low rejection efficiency of particulates) and GDM (i.e., low rejection efficiency of organics) processes. The GDM process showed higher removal rates of microplastics and larvae than the GAC process (i.e., 77.9% and 100% vs. 16.6% and 70%, respectively), and the GAC process exhibited higher removal rates of organic matter and perfluorinated compounds (PFOA and PFOS) than the GDM process (i.e., 54.8%, 90.9% and 99.1% vs. 17.6%, 23% and 31.8%, respectively). In the GAC-GDM hybrid system, stable water flux was observed with the efficient removal of CECs and organic matter during operation. This study implies that the GAC-GDM system can be used as a distributed water treatment system in remote areas such as islands and mountains because the GAC-GDM system is able to minimize the operation scale.

- **Keywords:** Gravity-driven ceramic membrane; Granular activated carbon; Microplastics; Perfluorinated compounds; Chironomidae larvae

Yuan Li, Chen Zhang, Yunsong Yu, Zaoxiao Zhang. *Design and optimization of VOC control process for tail gas in Rectisol unit based on steady state and dynamic simulation*. Pages 820-832.

Rectisol wash process(RWP) is a common process in coal chemical purification unit. However, the CO2 product gas and tail gas in the RWP carries volatile organic methanol, which must be controlled to meet the environmental protection requirements. This work develops a steady and dynamic model for the process of water washing tower(WWT) by Aspen Plus, which is used in Rectisol wash tail gas treatment. The effects of the theoretical stage number(TSN) and desalting water flow rate(FRdw) of the washing tower on the methanol concentration in tail gas(cMET) are studied through sensitivity analysis. The optimized TSN and FRdw of WWT are 16 stages and 15 t/h, respectively. The cMET is 4.1 mg/Nm3 under the optimal condition. The internal structure of WWT is optimized. The design of the WWT is verified by the hydraulic results and dynamic process simulation. The results help to efficiently and conveniently implement the control of volatile organic methanol from RWP.

- **Keywords:** Volatile organic compounds; Rectisol wash; Aspen Plus; Sensitivity analysis; Dynamic response; Mathematical model

Abdulaziz Sami Qambar, Mohammed Majid Al Khalidy. *Prediction of municipal wastewater biochemical oxygen demand using machine learning techniques: A sustainable approach*. Pages 833-845.

This paper proposes an integrated framework of remote sensing and machine-learning techniques to predict municipal wastewater influent biochemical oxygen demand (BOD5) in wastewater treatment plants (WWTPs). The study compares the performance of several supervised machine-learning algorithms, specifically decision tree, random forest, adaptive boosting, gradient boost, and extreme gradient boosting algorithms, against the wastewater received by two WWTPs in South Kingdom of Bahrain. The gradient boost algorithm model obtained the best results, scoring 1.00 coefficient of determination (R2) and 0.08 mean absolute error (MAE) against Askar WWTP dataset. In addition, the developed model showed its applicability and robustness against Al Dur WWTP dataset scoring 0.95 R2 and 3.93 MAE. This study showed that empirically, using a manual sampling method to obtain developed model input feature readings, the duration of the results can be accelerated by 40 times compared to traditional laboratory procedures. As a result, the duration was reduced from five days to only three hours. On the contrary, using real-time sensors to obtain developed model input readings, BOD5 can be predicted in real-time. The proposed approach mitigates environmental risks and ensures an effective treatment process that meets the effluent quality parameters.

- **Keywords:** Biochemical oxygen demand; Effluent; Influent; Machine-learning; Sustainability; Wastewater treatment plant

Bing Wang, Chunyang Gao, Xingchun Li, Yuzhu Zhang, Tongxu Qu, Xianyuan DU, Jin Zheng. *Remediation of groundwater pollution by in situ reactive zone: A review*. Pages 858-871.

Establishing an in situ reactive zone (IRZ) is an effective groundwater pollution remediation method that has been utilized extensively in actual contaminated sites. However, some controversial factors and technical bottlenecks hinder the establishment of an IRZ. For instance, we need to decide whether, under high pressure and high flow velocity, the colloidal remediation agent should be injected into the aquifer to increase or

reduce its migration ability. Additionally, methods need to be developed to monitor the diffusion range of colloidal remediation agents in the process of IRZ construction in real time and optimize the layout of injection wells. To clarify these uncertainties and resolve bottlenecks, this review first summarizes the development and design of IRZ technology to remedy contaminated groundwaters. Then, the types of colloidal remediation agents commonly used in IRZ technology are outlined, and the main mechanism of degrading pollutants is thoroughly analyzed. Additionally, the main mechanism of transport of colloidal remediation agents in aquifers is generalized. Finally, current knowledge gaps and future research prospects are identified and proposed. This review significantly improves our understanding of IRZ technology and provides valuable insights to researchers in this field.

- **Keywords:** In situ reactive zone (IRZ); Groundwater pollution; Colloidal remediation agents; Transport; Porous medium

Chunhua Zhang, Jinquan Chen, Xin Wu, Jiahui Shen, Dengming Jiao. *Poset-based risk identification method for rockburst-induced coal and gas outburst*. Pages 872-882.

The aim of this study was to address the problem of weighting disputes in the evaluation of rockburst-induced coal and gas outburst as well as to improve the rationality and accuracy of the risk identification results. Hence, we developed a risk identification method for rockburst-induced coal and gas outburst, considering the influence of multiple factors based on poset decision-making theory. The risk identification index system was established according to stress factors, gas factors, and physical and mechanical properties of coal, including 12 indexes and 4 risk grades. The poset adopted implicit weighting to store the weight information. The proposed method was applied to identify risks in an engineering case study. Thus, we determined the outburst risk grade and compared the case study results with the actual situation of the working surface. The comparison and analyses showed that the outburst risk grade of the case study working surface under gas factors was grade Ⅱ, the outburst risk grade under stress factors and the physical and mechanical properties of coal was grade Ⅲ, and the outburst risk grade under comprehensive factors was grade Ⅲ. The results of the risk identification of rockburst-induced coal and gas outburst based on poset were consistent with the results obtained by the method used in the case study and the actual situation of the working surface. This study extends the methods for accurately identifying risks of rockburst-induced coal and gas outburst and facilitates the formulation of effective preventive measures.

- **Keywords:** Rockburst-induced coal and gas outburst; Poset decision-making; Implicit weighting; Risk assessment

Shiqi Mu, Xinglong Chen, Yuanfeng Luo, Jingjing Zhang. *Degradation of petroleum hydrocarbons in oil-based drilling cuttings by a zero-valent iron Fenton-like advanced oxidation system*. Pages 883-891.

Oil-based drilling cuttings (OBDCs) containing large amounts of petroleum hydrocarbons generated from shale gas extraction constitute hazardous waste. In this study, the commonalities and differences of three systems, Fe0/peroxymonosulfate (PMS), Fe0/peroxydisulfate (PDS), and Fe0/H2O2, for treating OBDCs have been compared. The results show that oxidant initial concentration, Fe0 dosage, and reaction time are significantly positively correlated with the oil removal efficiency within certain ranges. Moreover, the initial pH is more critical in the Fe0/H2O2 and Fe0/PMS systems than in the Fe0/PDS system, with the oil removal efficiency being better under acidic conditions. FTIR and GC-MS analyses have shown that all three systems are effective in the removal of straight-chain alkanes, and the degradation ability decreases in the order Fe0/H2O2

> Fe0/PMS > Fe0/PDS. By characterizing the morphology, elemental composition, and crystal composition of OBDC before and after treatments, it showed that Fe0 was corroded and produced Fe2+, which benefited the formation of hydroxyl and sulfate radicals by reacting with oxidants (H2O2/PMS/PDS) and was responsible for the degradation of petroleum hydrocarbons of OBDCs. This study may provide theoretical support for the development and optimization of a technology for rendering OBDCs harmless.

- **Keywords:** Oil-based drilling cuttings; Advanced oxidation system; Zero-valent iron; Petroleum hydrocarbons

Hussein Abdelraouf, Jing Ding, Jiayi Ren, Guanshu Zhao, Fanyang Zhou, Shuyan Guan, Xuedong Zhai, Qingliang Zhao. *Gd-BiVO4 photocatalyst for organic contaminants removal: Short-term synthesis at sub-100 °C and enhanced sunlight-driven photocatalytic activity*. Pages 892-906.

A novel and short-term preparation method was conducted to fabricate pristine BiVO4, and Gadolinium (Gd) doped BiVO4 photocatalysts at sub-100 °C. The optical, structural, morphology, microstructure, and compositional characteristics of the fabricated photocatalysts were examined, which illustrated that the doping of Gd stabilized the existence of the tetragonal phase structure and enlarged the specific surface area of the pristine BiVO4. The comparison of the photocatalytic performance, preparation power consumption, and preparation cost showed the superiority of Gd doped BiVO4 photocatalyst fabricated by the Short-Term Synthesis Method at sub-100 °C. The ofloxacin (OFL) removal rate with 5%, 7%, and 10% Gd-BiVO4 photocatalysts was 1.53, 1.61, and 1.83 times that with pristine BiVO4 under sunlight, respectively. The degradation performance of target contaminants, including diclofenac, tetracycline HCl, ofloxacin, rhodamine B, and sulfadiazine, was demonstrated after one hour of sunlight irradiation with 5% Gd-BiVO4, achieving the removal efficiencies of 98.63%, 98.07%, 97.98%, 92.09%, and 78.56%, respectively. The effect of various factors on the removal performance was revealed, indicating that SO42− and H2PO4− had a remarkable inhibitory effect on the degradation. The 5% Gd-BiVO4 also showed excellent reusability and stability after five-cycle runs. The photogenerated holes (h+) and the superoxide radicals (•O2−) were the predominant generated active species, and the possible photocatalytic mechanism for the degradation of organic contaminants was proposed. Simple prepared Gd-BiVO4 photocatalysts were revealed to be a practical and potential choice for efficiently degrading contaminants with sunlight as green energy.

- **Keywords:** Gd doped BiVO4; Photocatalytic degradation; Short-term preparation method; Sunlight; Photocatalytic mechanism

Behrad Farzinfar, Farhad Qaderi. *Synergistic degradation of aqueous p-nitrophenol using DBD plasma combined with ZnO photocatalyst*. Pages 907-917.

In this study a dielectric barrier discharge non-thermal plasma (DBD-NTP) reactor was combined with ZnO nanoparticles to degrade p-nitrophenol (PNP) in aqueous solution. When the plasma process was combined with ZnO nanoparticles an obvious improvement was obtained in PNP removal efficiency. this was seemingly due to activation of ZnO photocatalysts under the UV light produced in discharge region. The results showed that addition of the optimum amount of ZnO nanoparticles (250 mg/L) to the plasma reactor could increase the removal efficiency from 49 % to 91 %, whereas the UV/ZnO photocatalytic process alone only lead to 12 % PNP removal. This is indicative of the synergistic enhancement of PNP degradation efficiency in the combined NTP-ZnO process rather than simply an additive effect. The effects of intial solution pH, applied voltage, and initial PNP concentration were also investigated on the sole NTP and NTP-ZnO

processes in terms of removal efficiency. Alkaline solution conditions, and lower initial PNP concentration favored both processes, while the applied voltage of 13 kV yielded the optimum PNP removal. Furthermore, higher total organic carbon (TOC) removal and higher kinetic constant of PNP degradation was achieved in the plasma system coupled with ZnO photocatalysis. Energy consumption analysis revealed that the NTP-ZnO process is 4.25 times more energy efficient than the sole plasma process which could be a major step towards industrial utilization of plasma treatment technologies.

- **Keywords:** DBD plasma; Photocatalysis; ZnO; P-nitrophenol

Bingchun Liu, Zhaoyang Han, Jin Li, Bo Yan. *Comprehensive evaluation of municipal solid waste power generation and carbon emission potential in Tianjin based on Grey Relation Analysis and Long Short Term Memory*. Pages 918-927.

With the rapid development of China's economy, the contradiction of the mismatch between municipal solid waste disposal capacity and its growth has become increasingly prominent, and the need to develop alternative energy sources has become increasingly urgent. Municipal solid waste incineration plays an important role in waste management. In this study, the Grey Relation Analysis (GRA) and Long Short Term Memory (LSTM) prediction model is constructed to achieve effective prediction of municipal solid waste generation by taking 11 influencing factors of municipal solid waste generation as input indicators in Tianjin. Meanwhile, this study predicts the power generation from municipal solid waste incineration and carbon emissions in Tianjin based on the prediction results. The experimental results show that the mean absolute percentage error (MAPE) value of the combined GRA-LSTM model established in this study is 6.759 %, and this model outperforms the other five structural methods in terms of prediction performance. By 2025, the amount of MSW in Tianjin will reach 3.74 million metric tons, the power generation through incineration will be 20.02–39.47 GWh, and the CO2 emission through incineration will be about 1.14 million metric tons. Finally, to cope with the growth of municipal solid waste generation and unbalanced power supply structure in the country's mega-cities, this paper puts forward relevant suggestions for achieving sustainable urban development.

- **Keywords:** Municipal solid waste, Long Short Term Memory, Waste-to-energy; Carbon emission

Zahra Sheikholeslami, Majid Ehteshami, Sara Nazif, Atieh Semiarian. *The environmental assessment of tertiary treatment technologies for wastewater reuse by considering LCA uncertainty*. Pages 928-941.

Tertiary treatment methods can result in severe environmental impacts that should be taken into consideration when deciding about the best system for wastewater reuse applications beside technical and economic issues. Life cycle assessment (LCA) commonly is used for evaluating the environmental impacts of these methods. Given the importance of uncertainty analysis, it is still an uncommon practice in LCA researches in recent years, especially those focused on tertiary wastewater treatment technologies (TWWTTs). Therefore, the main purpose of this study is to investigate the parameter and input data uncertainty in LCA of TWWTTs. Considering huge amount of data collected for LCA from different sources with various precision, there is high uncertainty in obtained LCA results that could affect the ranking of different methods based on their environmental impacts. The Monte-Carlo based method is used for uncertainty analysis of LCA and it is investigated how it can affect the final ranking of tertiary treatment methods based on their environmental impacts. In present study, LCA is used to study the environmental impacts of 22 tertiary treatment systems used for further treatment of effluent of South of Tehran wastewater treatment plant (WWTP) located at the south of Tehran, Iran. The

treated wastewater of this WWTP is planned to be used for different purposes including landscape irrigation and groundwater recharge as well as industrial and non-potable household (toilet flushing) usages. Among the 22 tertiary treatment systems, the best system for each application was chosen, based on the LCA results and the uncertainty of LCA.

- **Keywords:** Uncertainty analysis; LCA; Tertiary treatment system; Wastewater reuse; Environmental impacts

Mohammadreza Malekli, Alireza Aslani. *A novel post-combustion CO2 capture design integrated with an Organic Rankine Cycle (ORC)*. Pages 942-952.

Fossil fuel-based power plants are the significant sources of CO2 emitted into the atmosphere that significantly affect global warming. While these power plants provide the robustness of the grids, even with the fast development of renewable electricity, utilization of CO2 Capture and Storage (CCS) technologies is one of the best solutions to reduce their emissions and environmental risks. However, one of the most significant drawbacks of these technologies is their highest costs related to their energy consumption as well as the specific requirements of the solvents, which prevalently impact their adaptation. Among these technologies, Post-Combustion CO2 Capture (PCC) processes are widely used in the case of the power plant. This research develops an onshore Aqueous Post-Combustion CO2 Capture (APCC) process with water as a physical solvent to achieve a high CO 2 capture ratio with low energy consumption. The flue gas stream from a power plant flows into APCC, which can capture 72 kton/year of CO2. About 97.4% of CO2 was captured in the process with a 49.5% electricity production to consumption ratio (22.74 MWh/ton CO2) The captured CO2 is then delivered into a CO2 injection well to be used for Enhanced Oil Recovery (EOR) purpose with 15Mpa, 30 °C, and 80 mol% purity. Two scenarios were considered to decrease the external power requirements (1) the electricity production to consumption ratio is increased to 58.2% by adding a Hydro-Pump to the process; (2) coupling an Organic Rankine Cycle (ORC) with R125 working fluid to the process and using sensitivity analysis to gain the best thermodynamic conditions to increase the power production to consumption ratio to 80%. By considering both scenarios, the parasitic power is decreased by 52.78–28.44% and the net power production from the NGCC power plant is increased to 18.604 MW. Finally, Pinch Design Method (PDM) is used to reduce the Operating Cost of the process by the best utility selection from 2.48 M$/year to 0.945 M$/year, and the best Heat Exchanger Network (HEN) design in terms of the lowest Capital Cost at 4.71 M$/year was designed.

- **Keywords:** Aqueous Post-Combustion CO2 Capture; Hydro-Pump; Organic Rankine Cycle; Process Simulation; Pinch Design Method

Zhengqing Lin, Zhengwei Hu, Jingchao Peng, Haitao Zhao. *Dynamic-scale graph neural network for fault detection*. Pages 953-970.

Traditional graph-based dynamic fault detection methods describe the dynamic characteristic through constructing a single neighborhood graph at the current sample with some history samples. However, they ignore the diversity of dynamic properties of the variables in complex chemical processes. To overcome this problem, a novel neural network structure combining multiscale subgraphs is proposed, named dynamic-scale graph neural network (DSGNN), which divides variables into multiple groups according to their dynamic properties. DSGNN constructs a subgraph in each group. In traditional graph-based methods, the scale of the graph is usually manually designed. In DSGNN, the scale of each subgraph is decided by the dynamic properties of the variables in this subgraph. To aggregate the dynamic information, DSGNN utilizes convolution operations. The weights assigned to the neighbors in each subgraph are determined according to the

similarity between the current data and its neighbors. Low-dimensional features are extracted through the back-propagation technique from the updated high-dimensional features produced by convolution operations. Two case studies on a multivariate dynamic process and the Tennessee Eastman process are conducted to show the superiority of DSGNN.

- **Keywords:** Process monitoring; Fault detection; Dynamic feature extraction; Dimension reduction

Shilin Zhao, Junlin Peng, Runqi Ge, Kaibo Yang, Siyu Wu, Yuxin Qian, Tianle Xu, Junjie Gao, Yijun Chen, Zhiqiang Sun. *Poisoning and regeneration of commercial V2O5-WO3/TiO2 selective catalytic reduction (SCR) catalyst in coal-fired power plants*. Pages 971-992.

The NOx emitted from coal combustion can cause great harm to the environment and human health. The selective catalytic reduction (SCR) deNOx technology is a mature commercial deNOx technology, of which the SCR catalyst is the core. In China, the SCR deNOx technology has covered almost every coal-fired power plant since the 13th Five-Year Plan. Due to the complex and harsh working environment at the operating site, these catalysts will face the deactivation and replacement. This paper presents a comprehensive and systematic review of commercial V2O5-WO3/TiO2 SCR catalyst from three aspects, including composition and deNOx characteristics, poisoning, and regeneration, based on studies published in the recent years. It has an important guiding significance for the poisoning study and regeneration technology development of commercial SCR catalysts.

- **Keywords:** Coal-fired flue gas; Commercial SCR catalysts; V2O5-WO3/TiO2; Poisoning; Regeneration

Yingzi Lin, Jing Chen, Mingliang Zhou, Gen Liu, Siwen Li, Chunyan Shi, Mengshi Wang, Shenglin Qi. *Efficiency and mechanism of zero-valent iron/nitrilotriacetic acid/peroxymonosulfate system for degrading sulfamethazine*. Pages 993-1008.

In this paper, the efficiency and mechanism of using nitrilotriacetic acid(NTA) as a complexing agent to enhance the zero-valent iron(Fe0)/peroxymonosulfate(PMS) system to remove sulfamethazine(SMZ) from water are discussed. Research results show that the addition of NTA increases the soluble iron by 3.05 times, and the decomposition rate of PMS increases from 27% to 62%. Keeping other conditions unchanged and increasing the concentration of PMS to 0.2 mM, the degradation rate reaches the peak, continued increase of PMS concentration will decrease the degradation rate. The degradation rate of SMZ is positively correlated with Fe0 concentration. The effect of different inorganic ions on the degradation of SMZ was investigated. The high concentration of Cl− promoted the degradation effect, and the reaction rate constant of the system is increased by 1.67 times when the Cl− dosing is 10 mM. The PMS/Fe0/NTA system degrades SMZ up to 79.36% in actual water bodies. The degradation of SMZ is mainly by Smiles-type rearrangement, sulfonamide bond breaking, etc. The toxicity test proves that the inhibition rate of luminescent bacteria before and after degradation decreases from 61.86% to 40.47%, with an overall decreasing trend of toxicity.

- **Keywords:** Peroxymonosulfate; Zero-valent iron; Nitrilotriacetic acid; Sulfamethazine; Degradation; Degradation mechanism

Lingqing Wang, Xueping Wang. *A holistic assessment of spatio-temporal pattern and water quality in the typical basin of northeast China using multivariate statistical methods*. Pages 1009-1018.

The deterioration of water resources has been recognized as an urgent environmental problem due to population growth, industrialization, urbanization and agricultural activities, where water quality assessment is the basis for forward-looking decisions on water quality management. In this study, the Nemerow index method, traditional fuzzy mathematics and improved fuzzy mathematics methods were applied to assess the water quality of the Liao River based on twenty-three water quality parameters. The results revealed that most monitoring stations in the study area were moderately polluted. The improved fuzzy mathematics method gives more appropriate than the other two methods in water quality assessment. The self-organizing map (SOM) results suggested that chemical oxygen demand (CODCr) significantly affects water quality. The human health risk model was applied to calculate hazard indices (HI) to assess human health risks, indicating that the health risk of the Liao River caused by heavy metals was within an acceptable limit and did not pose a significant human health risk in the study area. Meanwhile, the health risk caused by heavy metals to children was higher than in adults. The results of the present study could provide new insights into water quality assessment, risk warning and public health protection in typical urbanized watersheds.

- **Keywords:** Water quality assessment; Water quality index; Self-organizing map; Improved fuzzy mathematics; Human health risk assessment

Hujun Li, Hongxiao Wu, Zhen Wang, Guokai Zhang, Jie Li, Hang Zhou, Mingyang Wang, Yong He. *Experimental and numerical simulation of the propagation law of shock waves in corrugated steel-lined tunnels*. Pages 1019-1030.

Corrugated steel support structures are widely used in engineering tunnels owing to their rapid construction and high bearing performance, allowing for the complex propagation of shock waves. To clarify the propagation law of shock waves in a corrugated steel tunnel with interior lining, a 30-m-long straight tunnel was built to explore the propagation of an explosion shock wave, and three different tunnel inner walls were designed, namely, a concrete inner wall and two types of corrugated steel linings. Based on the data on the monitored shock wave, the propagation law of shock waves in the tunnel was obtained, and the influence of corrugated steel linings on the shock waves was analyzed. A finite element model of the channel was established to verify the results of experiment and determine the model and related parameters. This model was also used to perform a numerical simulation of explosion shock wave propagation in corrugated steel-lined tunnels of various sizes. Based on the experimental and numerical simulation results, a prediction model of shock wave overpressure in corrugated steel-lined tunnels was obtained. Research showed that the shock-wave energy of wavefronts near walls was diverted, the formation and propagation of waves reflected from walls was affected by corrugated steel linings, which effectively improved the attenuation efficiency of shock waves in tunnels.

- **Keywords:** Shock wave; Corrugated steel structure; Propagation law; Decaying mechanism

Ling Ding, Bowei Chen, Yan Wang, Yong Zhang. *High efficiency adsorption of uranium in solution using nano-TiO2 loaded with g-C3N4*. Pages 1049-1057.

In this study, g-C3N4 was used to load with nano-TiO2 (NT) to prepare g-C3N4 @NT with good dispersibility in aqueous solution for the separation of uranium(VI) from

wastewater. The adsorption efficiency for uranium(VI) by g-C3N4 @NT reached 90 % within 30 min and the maximum adsorption capacity for uranium(VI) on g-C3N4 @NT was 557.4 mg g−1, which was significantly better than that of NT (270.3 mg g−1). The studies of isotherm model and kinetic model indicated that the adsorption process to uranium(VI) on g-C3N4 @NT was a single-layer chemisorption process. The interaction mechanism between uranium(VI) and g-C3N4 @NT was further proved by SEM and XPS, which was attributed to the filling of oxygen vacancies, the oxidation-reduction effect and the inner spherical surface complexation. The results showed that g-C3N4 @NT might be expected to be used in removing uranium(VI) in solution.

- **Keywords:** Titanium oxide; G-C3N4; Adsorption; Uranium

Rizwan Ahmad, Muhammad Aslam, Guo Jing, Daeeun Kwon, Jeonghwan Kim. *Comparison of pyrophyllite- and alumina-coated membrane treating industrial wastewater in aspect of membrane fouling and organic removal*. Pages 1058-1066.

In this study, two ceramic membranes such as coated alumina-based (ACA) and low cost coated pyrophyillite-based (ACP) membranes were compared for elucidating the effect of feed charge on fouling control and fluidization of adsorbent on the treatment of organic solution. The granular activated carbon (GAC) was fluidized along the surface of ceramic membrane to provide physical scouring and adsorption capability. Results revealed that the surface of ACP membrane was rougher than that of ACA membrane showing surface roughness of 81.2 and 61.6 nm, respectively. Furthermore, contact angle of ACP membrane was higher than that of ACA membrane (32° vs. 10°). Without GAC fluidization, the fouling rate resulting from ACP membrane was dependent upon the type of wastewater. With ACP membrane, membrane fouling was higher with cationic dye-based wastewater than that with anionic dye-based one. Regardless of different types of wastewaters, relatively low fouling was observed for ACA membrane. The intrinsic properties of membranes such as surface roughness, surface charge and hydrophilicity played important roles in determining membrane fouling. Low organic rejection efficiency (less than 40 %) was observed during membrane filtration without GAC. However, almost 98 % of organic rejection efficiency was reached within initial 30 min of filtration under the GAC fluidization at 50 % of packing ratio based upon effective reactor volume. Under the 10 % of packing ratio with GAC particles, membrane fouling was controlled successfully during 12 h filtration with almost complete UV removal efficiency within initial 4 h of filtration.

- **Keywords:** Adsorption; Membrane fouling; Wastewater; Ceramic membrane; Morphology

Osama Abrahiem AL Falahi, Siti Rozaimah Sheikh Abdullah, Hassimi Abu Hasan, Ahmad Razi Othman, Hind Mufeed Ewadh, Setyo Budi Kurniawan, Muhammad Fauzul Imron. *Occurrence of pharmaceuticals and personal care products in domestic wastewater, available treatment technologies, and potential treatment using constructed wetland: A review*. Pages 1067-1088.

Contaminants of emerging concern (CECs) are primarily anthropogenic compounds found in water at trace concentrations and mostly still ignored. Pharmaceuticals and personal care products (PPCPs) are two popular categories of CECs. PPCPs are persistent in the environment and capable of disrupting the physiology of target receptors. PPCPs are reported to be overused daily and exposed to aquatic environment via multiple routes, including municipal and industrial effluent. Nevertheless, there is a lack of a comprehensive summary of PPCPs removal techniques, particularly in wastewater treatment plants (WWTPs). While WWTPs are inefficient at removing PPCPs, they serve

as primary barriers to the spread of CECs. This paper reviews and highlights the conventional treatment technologies involved for PPCPs removal in WWTPs as well as comparison with phytotechnology in the wastewater treatment field to combat the disconcerting occurrence of PPCPs. Operating parameters in applying phytotechnology, including retention time and aeration requirement as well as major challenges for phytoremediation of PPCPs are evaluated. Fate of PPCPs (focused on ibuprofen and paracetamol) are discussed in detail during treatment using constructed wetland. The results validated concerns regarding the prevalence of PPCPs and the good potential of using constructed wetland as tertiary treatment in WWTP to avoid further spreading of PPCPs to the environment.

- **Keywords:** CEC; Constructed Wetland; Environmental pollution; Ibuprofen; Paracetamol; Pharmaceutical

Yiming Jiang, Xuhai Pan, Qiong Cai, Oleksiy V. Klymenko, Min Hua, Tao Zhang, Zhilei Wang, Qingyuan Wang, Andong Yu, Juncheng Jiang. *Effects of the partially open inlet on shock waves and spontaneous ignition during the leakage of hydrogen*. Pages 1089-1100.

Unexpected spontaneous combustion and shock waves can occur when high-pressure hydrogen leaks into pipelines, whilst irregular leakage ports affect their features. In this paper, shock waves and self-ignition are experimentally and numerically studied after the pressurized hydrogen is released through the partially open inlet. And the effects of tube length and release pressure are investigated. Pressure signals, light signals, and flame images are used to characterize the shockwave, self-ignition, and flame propagation. Results show that the shock-affected region can be formed near the partially open inlet. It is accompanied by complex wave structures, shock wave interactions, and shock wave focusing. The contact surface is distorted and deformed. The flow field parameters near the inlet change dramatically and are unevenly distributed, which affect the overpressure characteristics recorded by the pressure sensors. The initial intensity of the shock wave is lower than that in tubes with the fully open inlet at the early stage of the leakage. In addition, the partially open inlet influences the critical pressure at which spontaneous ignition occurs and the flame evolution inside or outside the tube. It has an inhibition effect on spontaneous ignition, but this inhibition effect weakens with increasing tube length.

- **Keywords:** Hydrogen safety; Leakage; Partially open inlet; Shock wave; Spontaneous ignition

Ritesh Krishna Sambare, Satish Kumar Dewangan, Pankaj Kumar Gupta, Sandeep Joshi. *Energy, exergy and economic analyses of tubular solar still with various transparent cover materials*. Pages 1101-1108.

In order to use solar energy to convert raw ground and surface water into clean potable water, several distillation systems have been investigated so far. However, to be sustainable, the productivity of these systems must be as high as possible. Tubular solar stills (TSS) were investigated as one of the more productive solar distillation systems. The current study aims to improve the productivity of tubular solar stills by exploring different cover materials. The experimental study was carried out on four different TSS setups with cover materials made of polyvinyl chloride (PVC), polycarbonate, acrylic, and glass. In comparison to other materials, it has been observed that the TSS with glass cover gives the maximum productivity (6.23 L/m2) and daily exergy and energy efficiency (7.67%, 71.56%, respectively) for the same water depth of 0.5 cm in each basin. According to the economic analysis of all the arrangements carried out, the TSS with Acrylic cover provides the lowest cost of producing freshwater among all of the investigated combinations.

- **Keywords:** Tubular solar still; Tubular transparent materials; Energy analysis; Exergy analysis; Economic analysis; Productivity enhancement

Lixu Wu, Jun Hu, Chun Sun, Feipeng Jiao. *Construction of Z-scheme CoAl-LDH/Bi2MoO6 heterojunction for enhanced photocatalytic degradation of antibiotics in natural water bodies*. Pages 1109-1119.

Heterojunction construction is considered to be an effective method for improving photocatalytic efficiency. Herein, Z-scheme heterojunction CoAl-LDH/Bi2MoO6 was synthesized by a simple hydrothermal method. Due to the strong hydrolysis ability of Bi3+ made the solution acidic, to prevent the solution of CoAl-LDH, the reaction solution was adjusted to neutral by NaOH solution. The prepared materials were characterized by a series of analytical techniques and their photocatalytic performance was evaluated by photocatalytic degradation of antibiotics under natural aqueous conditions (seawater and the water from the Xiangjiang River). The composite with 10% CoAl-LDH (CBA-10) displayed the optimal degradation efficiency and still had good photocatalytic activity in seawater and Xiangjiang water compared to the pure water for degradation of antibiotics. According to the photoluminescence (PL) and electrochemical impedance spectroscopy (EIS) test results, the heterojunction formed between CoAl-LDH and Bi2MoO6 effectively promoted the separation and migration of electrons and holes, thus increasing the photocatalytic degradation efficiency. In addition, the degradation efficiency of the composite with 10% CoAl-LDH under pure water conditions was 85.98% and 72.69% for tetracycline and ciprofloxacin respectively after five cycles of testing, which showed that the composite with 10% CoAl-LDH had good stability and reusability. This work would contribute to the development of composite materials for photocatalytic degradation of contaminants in natural water bodies.

- **Keywords:** Removal of organic wastewater; Z-scheme CoAl-LDH/Bi2MoO6 heterojunction; Natural water bodies

Fanyi Meng, Paul Amyotte, Xiaochen Hou, Chang Li, Caodi He, Gang Li, Chunmiao Yuan, Yuntao Liang. *Suppression effect of expandable graphite on fire hazard of dust layers*. Pages 1120-1130.

Expandable graphite (EG) has potential to inhibit the fire hazard of dust layers. This suppression effect was systematically studied by comparing with that of traditional inertants such as CaCO3 and NaHCO3. The thermal expansion of EG can generate compact char layers with low thermal conductivity, which effectively inhibited the heat transfer between the heat source and the surrounding dusts. Oxygen diffusion was also hindered between the dust layer and the environment. Therefore, a small amount of EG could achieve a suppression effect for layer fires equivalent to a large amount of traditional inertants. A small amount of traditional inertants promoted the combustion of the non-metal dust layer, a phenomenon that did not occur while using EG. In addition, EG also acted as an effective flame retardant on the flame spread of the non-metallic dust layer under inclined conditions. Most important, EG had a suppression effect on down-flowing moving pool fires of non-metallic dust layers and the violent combustion of metal dust layers. This shows great potential not available in traditional inertants. EG could be considered as a novel and well-integrated dust layer fire inhibitor in process industries handing combustible dusts.

- **Keywords:** Expandable graphite; Dust layer; Fire hazard; Suppression mechanism

Márcio Daniel Nicodemos Ramos, Gabriel Lira Santana Silva, Tomás Lemos Lessa, André Aguiar. *Study of kinetic parameters related to dyes oxidation in ascorbic acid-mediated Fenton processes*. Pages 1131-1141.

Ascorbic acid (AA) is a natural reducer that has been used as a prooxidant additive to improve dyes oxidation via Fenton processes (Fe2+/H2O2 and Fe3+/H2O2). In the present work, low concentration of AA (10 μmol L1) enhanced Bismarck Brown Y (BBY), Safranin T (ST), Rhodamine B (RB), and Reactive Black 5 (RB5) decolorizations in solution, mainly in reactions initially containing Fe3+ as a catalyst (Fe3+-reactions), e.g., Fe3+/H2O2 decolorization of RB5 was increased from 54 % to 73 % after 60 min due to added AA. Decolorization increased from 0 up to 60–90 μmol L−1 of added reducer. At higher concentrations, AA did not improve decolorization. The dyes were decolorized below 10 % when incubated with 1 % tert-butanol, indicating that HO• radical is the main oxidant involved in the reactions. The kinetic analysis showed that the 1st- and 2nd-order kinetic models fitted well to both Fe2+- and Fe3+-reaction data. The BMG kinetic model also fitted well to the Fe2+-reactions (with and without AA), along with Fe3+/H2O2/AA. Based on these kinetic models, we verified that reaction rate constants were increased due to added AA. There was a decrease in activation energy (Ea) in decolorizing ST from added AA by varying the reaction temperatures. For example, Ea decreased from 111.6 to 81.8 kJ mol−1 for Fe3+-reactions and from 72.6 to only 69.3 kJ mol−1 for Fe2+-reactions. The AA/H2O2 system was least effective in decolorizing ST since Ea was 130 kJ mol−1. In summary, ascorbic acid decreases the energy barrier to improve Fenton-based ST oxidation.

- **Keywords:** Fenton reaction; Ascorbic acid; Textile effluent; Kinetics; Hydroxyl radical

Fang Yan, Longjun Dong, Bing Wang, Ji Ge, Ben Wang. *Using risk meshing to improve three-dimensional risk assessment of chemical industry*. Pages 1166-1178.

With the development of three-dimensional (3D) risk assessment, the accuracy of 3D risk calculations plays an important role in ensuring the quality of risk assessment results for the chemical industry. A more accurate risk calculation is significant to improving the accuracy and reasonability of 3D risk assessment results. Therefore, a novel risk calculation method called risk meshing (RM) for field theory-based 3D risk assessment is proposed in this study. For the proposed RM, the 3D risk is evaluated and calculated based on the possibility, vulnerability, and consequence with respect to the risk. An assessed elementary unit (AEU) is then introduced to compute the 3D risk in different partitioned blocks by taking advantage of the regional evaluation ability with respect to the vulnerability assessment. Fire and explosion accidents caused by storage tanks in a coal chemical industry plant are employed to make a case study, and the evaluation results show that RM can provide more accurate results because building and road layouts are considered for the risk calculation. Meanwhile, the optimal risk reduction route (ORRR) is confirmed by RM and using traditional methods. Hence, the validity of RM is verified based on the comparison of ORRRs obtained by RM and those by traditional methods. The paper indicates the significance of RM in improving the accuracy and reasonability of 3D risk assessments by analyzing the evaluation and comparison results, which lays a theoretical foundation for further development of field theory-based 3D risk assessments of chemical industry.

- **Keywords:** Three-dimensional risk assessment; Field theory; Risk calculation; Assessed elementary unit; Vulnerability assessment; Chemical Industry

Zhaohui Zhang, Jing Wu, Lin Shao, Liang Wang, Xiaoming Yang, Bin Zhao, Junjing Li, Cong Ma, Xiuru Chu, Pengda Zhang. *Comparison*

***between integrated MIEX/UF and PAC/UF in long-term irreversible membrane fouling reduction: Effectiveness and mechanism analysis*. Pages 1179-1187.**

In an integrated adsorption/ultrafiltration process, the choice of adsorbent is key as it affects the effluent water quality in addition to providing membrane fouling control. Magnetic ion-exchange resin (MIEX) and powdered activated carbon (PAC), two of the most used adsorbents in water treatment processes, have similar organic matter removal abilities. However, the corresponding integrated processes exhibited significant differences in terms of irreversible membrane fouling mitigation. Long-term filtration experimental results suggested that the chemical cleaning interval of the MIEX/UF process was 134% longer than that of the PAC/UF process. In addition, MIEX/UF had a 28.8% reduction for the chemically irreversible fouling rate compared to that of PAC/UF. Hydraulically irreversible fouling was effectively alleviated in the MIEX/UF process throughout long-term operation, whereas fouling was exacerbated in the PAC/UF process under the condition of timed chemical cleaning. Further analysis indicated that in the PAC/UF process, irreversible fouling control depended on adsorption; however, fouling mitigation in the MIEX/UF process mainly relied on the enhancement of backwashing by the MIEX dynamic layer. The significant difference in the interfacial forces between the MIEX-pollutants and PAC-pollutants was the fundamental cause for this phenomenon. Therefore, the mitigation of membrane fouling in an integrated adsorption/UF process depends more on the adhesion force between the adsorbent and pollutants than on the adsorption capacity of the adsorbent.

- **Keywords:** MIEX; Irreversible membrane fouling; Powdered activated carbon; Ultrafiltration; Micro-interfacial force

Purusothmn Nair S Bhasker Nair, Raymond R. Tan, Dominic C.Y. Foo, Michael Short. *A process integration-based multiperiod energy planning model for CO2-intensive industries*. Pages 1188-1200.

Multiperiod carbon-constrained energy planning considers long-term demand variations as well as progressively stringent CO2 emission limits towards net-zero carbon goals. Previous work on multiperiod energy planning has predominantly focused on the power generation sector. Nevertheless, emissions originating from industries must be mitigated to achieve decarbonisation at different (e.g., corporate, national, or regional) scales. This work develops a multiperiod energy planning model to determine the optimum deployment of energy sources for CO2-intensive industries other than the power generation sector. A hybrid approach is employed in this work, making use of the combined automated targeting model (ATM) and superstructure models. The hybrid approach in this work overcomes the non-linearity in the CO2 intensity calculations. Solving the ATM and superstructure model simultaneously ensures that both demand and CO2 emission limits for all industries are satisfied in each period. The multiperiod energy planning model is demonstrated with a case study with and without CO2 load transfer scenarios. The case study is performed for 21 industries across three 5-year periods. For the CO2 load transfer scenarios, the CO2 emission limits may be violated in earlier periods, triggering CO2 debts. The latter are compensated by CO2 credits in later periods where the total CO2 load is below the emissions limit due to aggressive mitigation strategies. Alternatively, in the absence of CO2 load transfer, the CO2 emission limits for all periods must be satisfied. Results show that the deployment of low-carbon energy sources (e.g., biomass and biogas) is necessary for the satisfaction of the CO2 emission limits within each period. Once CO2 capture and storage (CCS) is available, its deployment would complement existing mitigation strategies in later periods. The deployment of CCS on power plants fueled by biomass and biogas make them as negative emissions technologies (NETs) which are useful for CO2 removal (CDR). The development of the multiperiod energy planning model in this work allows

decarbonisation strategies to be simultaneously employed across all industries for a cumulative CO2 emissions reduction.

- **Keywords:** Negative emission technologies (NETs); Carbon emissions pinch analysis (CEPA); CO2 Capture and Storage (CCS); Renewable energy sources; Automated Targeting Method (ATM); Superstructure model

Marco F. Paucar-Sánchez, Mónica Calero, Gabriel Blázquez, Rafael R. Solís, Mario J. Muñoz-Batista, M. Ángeles Martín-Lara. *Thermal and catalytic pyrolysis of a real mixture of post-consumer plastic waste: An analysis of the gasoline-range product*. Pages 1201-1211.

In this work, the thermal and catalytic pyrolysis of different types of plastic waste and a real mixture were investigated in a fixed-bed reactor over different catalysts (CaO, MgO, HY, HZSM-5). Important differences in gas, liquid, and solid yields were found as a function of polymer type. The highest gas yield was obtained with expanded polystyrene (52.3%), and the maximum oil production with high-impact polystyrene (55.5%), while polypropylene film led to the highest char release (17.5%). Regarding the composition of the liquid oil, high-impact polystyrene showed the highest yield of gasoline-range product (426 g per kg of pyrolyzed plastic), mainly composed of aromatics compounds (90%). The addition of catalysts increased the gas yield to the detriment of the oil produced. The effect was more evident for zeolite-type catalysts, i.e., the gas yield raised from 43.3 (non-catalytic) to 51.5% (HZSM-5). Low influence on the oil composition, i.e., gasoline-range product, was detected. This can be explained by the fast deactivation of catalysts because of coke deposition. Only an increase in the fraction of gasoline in liquid oil was observed when low-cost catalysts (CaO and MgO) were used, without significant changes in the composition of this product.

- **Keywords:** Plastic waste; Pyrolysis; Catalysts; Gasoline-range product; Hydrocarbon types

Soham Dutta, Katie A. Mulligan, Brenton L. Drake, Kevin L. Simmons, Amy L. Koziol, Steven E. Horsch. *Is your ARC data misleading? Heat-transfer limitations and reaction rate underestimation in Accelerating Rate Calorimetry*. Pages 1212-1218.

Accelerating Rate Calorimetry (ARC) is a widely used adiabatic calorimetry technique to evaluate thermo-kinetics of hazardous chemical reactions. Most ARCs rely on measurement of temperature at the external wall of the ARC sphere to evaluate the temperature rise rate, and therefore exothermic reaction rate. We report large temperature gradients between the center and wall for a granulated solid sample tested using an un-stirred ARC that leads to varying spatiotemporal temperature profiles. Such gradients were found to be significantly lowered in organic liquid samples, enabling classifying some granulated solid samples as heat transfer-limited systems. This study reveals that such temperature gradients obviate estimation of representative exothermic reaction rate, manifesting in hazard underestimation through erroneous pressure and apparent conversion profiles. Next, the addition of an inert was demonstrated to reduce the magnitude of such gradients, thereby enabling relatively accurate hazard assessment and offering a potential solution. Lastly, several strategies are outlined to allow researchers to identify and mitigate the influence of gradients during hazard assessment. Researchers must be cognizant of the potential for gradients when analyzing and interpreting ARC data for thermo-kinetic modeling and hazard evaluation. During hazard evaluation, researchers should confirm that no significant gradients exist or find ways to de-sensitize their hazard assessment parameters if gradients exist and cannot be minimized.

- **Keywords:** Accelerating Rate Calorimetry; Exothermic; Thermal lag; Adiabatic; Calorimetry; kinetics; Hazard assessment

Shijin Zhang, Xiaowei Huo, Suzhou Xu, Yanting Zhang, Benyin Zhang, Mingming Wang, Qingguo Wang, Jing Zhang. *Original sulfur-doped carbon materials synthesized by coffee grounds for activating persulfate to BPA degradation: The key role of electron transfer*. Pages 1219-1234.

In this work, sulfur-doped (S-doped) carbon materials (SCs) were successfully synthesized by using coffee grounds which are relatively cheap and easily available. Results show that SCs exhibit excellent catalytic activity for persulfate (PS) activation and a more than 99% bisphenol A (BPA) degradation rate was achieved. Meanwhile, 82.3% of total organic carbon (TOC) can be removed in 40 min at 25 °C when applying a dosage of 0.15 g/L SCs and 1 mM PS under an initial pH of about 4.0. SEM and BET characterization methods were used to reveal the surface characteristics of the material. It is found that SCs had a porous structure and a specific surface area of 159.319 m2/g, which conferred to SCs superior adsorption (17.3 mg/g). Additionally, kinetic and adsorption isotherm models for adsorption by SCs were obtained via linear fitting, which proved that the process was better described by the pseudo-second-order model (R2 = 0.9989) and Langmuir model (R2 = 0.9890). The free radical quenching experiments, electron paramagnetic resonance (EPR), and open circuit potential (OCP) tests together demonstrated that the system achieved BPA degradation via non-radical pathways (singlet oxygen and electron transfer). It is speculated that S-doping is able to effectively promote electron transfer given the XPS results. Finally, batch control experiments were run to investigate the influence of PS concentration (0.2 – 2.0 mM), BPA concentration (0.005 – 0.03 mM), SCs dose (0.05 – 0.25 g/L), pH (4.0 – 10.0), and Cl− and HCO3− (1 or 5 mM) on the degradation of BPA. Evidently, the catalysts could be used for a wide range of BPA removal scenarios. In a word, S-doped carbon materials prepared from coffee grounds can improve the degradation of BPA and activation of PS under a wide range of operating conditions. Simultaneously it was strongly associated with electron transfer in non-radical pathways. This research lays the foundation for the rational design of a persulfate-based system for use as an actual water purification catalyst.

- **Keywords:** Carbon material; Sulfur-doped; Persulfate; Singlet oxygen; Electron transfer; Bisphenol A