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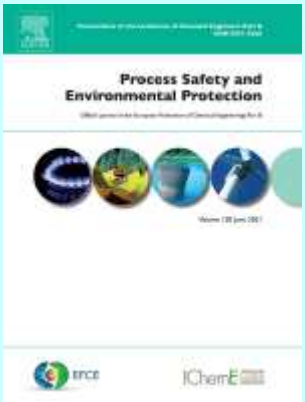

Ming Luo, Yanjun Qin, Jianjun Cai, Lili Qian, Shuxiang Wang, Haiyan Zhang, Lunzheng Zhou, Peng Liu. *Sulfur release and migration characteristics in chemical looping combustion of high-sulfur coal*. Pages 1-9.

Chemical looping combustion of coal has attracted great attention due to its advantage in carbon capture. Sulfur in coal may have negative impacts on this process including deteriorating the reactivity of oxygen carrier and generating gaseous sulfur species. In this research, the release and migration characteristics of sulfur in the chemical looping combustion of Xinzhou coal with two synthetic oxygen carriers, CuO/SiO2 and NiO/Al2O3, were investigated by experiments and thermodynamic simulation. The thermodynamic analysis showed that sulfur in coal mainly migrated to metal sulfides at lower temperatures and peroxide coefficients, but the formation of SO2 was favored at higher temperatures and peroxide coefficients. Experimental results showed that the sulfur conversion efficiencies (XS,g) during the reduction stage reached 62.34 % and 61.25 % under Cu- and Ni-based oxygen carriers, respectively, and XS,g during the reoxidation stage were 6.25 % and 7.44 %, respectively. For both oxygen carriers, the share of H2S and SO2 in the sulfurous gases exceeded 96 % during the reduction stage, while SO2 was the only sulfurous gas when air was introduced. Even though the metal sulfides (Cu2S, Ni3S2 and NiS) were observed in the reduced samples, those two oxygen carriers showed satisfactory regeneration performance after one redox process.

- **Keywords:** Chemical looping combustion; Sulfur; Oxygen carrier; Coal; CO2 capture

Fu-Rong Xiu, Ke Zhou, Xuan Yu, Yingying Qi. *Co-treatment of PVC and used LCD panels in low-temperature subcritical water: Enhanced dechlorination and mechanism*. Pages 10-19.

The dechlorination of polyvinyl chloride (PVC) and the removal of organic materials from used liquid crystal display (LCD) are the primary difficulties and steps in the safe disposal of these two types of waste. In this study, the dechlorination of PVC and the removal of organic materials from waste LCD were simultaneously accomplished by using a low-

temperature subcritical water (SubCW) co-treatment due to the low dielectric constant and mass transfer resistance of SubCW. The dechlorination efficiency of PVC could be significantly enhanced by introducing waste LCD in the SubCW co-treatment with lower PVC-to-H2O ratio (1:20 g/mL and 1:30 g/mL). The temperature, time, PVC-to-H2O ratio, and PVC-to-LCD ratio have significant influence on the dechlorination efficiency and chlorine distribution. The optimal parameters of the co-treatment were as follows: 220 °C, 90 min, PVC-to-LCD ratio of 4:1, and PVC-to-H2O ratio of 1:30 g/mL. In the optimal conditions, the PVC dechlorination efficiency could reach as high as 100 %. The removed chlorine was completely transferred to the aqueous phase and could be recovered as inorganic chlorine, eliminating the risk of chlorine. It is a remarkable improvement for the PVC dechlorination at low temperature with lower PVC-to-H2O ratio. The organic materials contained in used LCD could be efficiently removed by the SubCW co-treatment above 200 °C, and part of inorganic substances in used LCD could dissolve during the co-treatment due to the interaction between metallic oxides in LCD and HCl removed from PVC. The stable alkene-carbonyl structure (CCO) could be formed in the PVC residue during the SubCW co-treatment of PVC + LCD, promoting the dechlorination reaction of PVC. It is believed that the SubCW co-treatment is a high-efficiency strategy both for the dechlorination of PVC and the pre-treatment of used LCD.

- **Keywords:** Polyvinyl chloride; Used liquid crystal display; Low-temperature subcritical water; Co-treatment; Dechlorination

Xiyan Guo, Wei Tan, Liyan Liu, Cenfan Liu, Guorui Zhu. *Experimental study of liquefied gas dynamic leakage behavior from a pressurized vessel*. Pages 20-27.

The accidental releases of pressurized liquefied gases from tanks involve violent phase transformation, which would generate two-phase releases and flashing jets. To investigate the evolution of leakage behaviors and make an analysis of near-field jet flow characteristics, a small-scale liquefied gas release experiment has been established. Leakage holes with different length-diameter ratio (LDR) have been used to analyze interactions between the leakage holes and release behaviors. Morphological characteristics of jet expansion angles have been obtained by high-speed camera, and jet velocities have been measured by particle image velocimetry (PIV). Meanwhile, the depressurization process, variation of temperature in the tank and mass outflow rates were obtained. Results show that, despite the LDR is varying, expansion angles and jet velocities behavior in the same tendency: decreases in the initial and maintains in a stable value for a period. The stable velocity status was worked by the balanced pressure drop. Thereafter, an empirical two-phase mass outflow rate model is developed based on the experimental data, which is related to the nozzle geometric parameter and upstream pressure, 90 % of the experimental data are within ±12 % of the prediction. Therefore, the empirical two-phase model can be supported in the mass flow rate evaluation, especially for the release cases that LDR are smaller than 5.00 but larger than 2.00. The experimental data is beneficial for providing further insight into the prediction of accidental release and risk assessment for the liquefied gas transportation and storage.

- **Keywords:** Small scale release experiment; Flashing jet; Two-phase flow; Model validation; R134a

Huan Xu, Wangyong Jin, Jie Luo, Feng Wang, Hailin Zhu, Guojin Liu, Yuan Yu, Caihong Lei, Yuhai Guo. *Study of the PTFE multi-tube high efficiency air filter for indoor air purification*. Pages 28-38.

Particulate matter air pollution has become a severe environmental issue because it poses a great threat to human health. In this work, a new type of Polytetrafluoroethylene (PTFE) multi-tube high efficiency particulate air filter was successfully prepared by applying PTFE sheet membranes that wrapped the nonwoven tube for the improvement

of the indoor air quality. The properties and filtration performance of three types of PTFE sheet membranes were explored. The PTFE tubular membrane filters with different diameters, lengths and membrane layers were prepared and tested for the ability to remove particulate matter. The results revealed that the PTFE sheet membranes had excellent hydrophobicity and possessed the microstructure of nodes interconnected by fibrils. The thicker and smaller pore size membranes had higher efficiency, and the efficiency curves for the PTFE sheet membranes demonstrated the typical shape of a "V" from 10 to 300 nm at face velocities from 0.3–15 cm/s. The best type of tubular membranes in terms of diameter and length was dependent on the packing density and the height of the filter cavity. According to the test results, the filter contained two layers of membranes had the lowest pressure loss while achieving an ultra-high particle removal efficiency of over 99.98 % for particles (0.3 μm) and nearly 100 % for particles (2.5 μm). The fouling tendency in the staggered arrangement of tubes was less than that in the aligned arrangement. Therefore, the PTFE multi-tube air filter based on the sheet membrane might have a positive potential application for PM removal from air pollution.

- **Keywords:** PTFE sheet membrane; Tubular membrane; Air filtration; Fresh air; Efficiency; Indoor air

Liyan Liu, Yunhui Pang, Dong Lv, Kang Wang, Yang Wang. *Thermal and kinetic analyzing of pyrolysis and combustion of self-heating biomass particles*. Pages 39-50.

As a renewable fuel, the application of biomass fuel gets more and more attention. Fire and explosion are the main safety problems in the biomass fuel storage process. The characteristic parameters and kinetic analysis of pyrolysis and combustion are significant to guide the safe storage of biomass fuel. In this work, the thermogravimetric analysis (TGA) was used to obtain the pyrolysis and combustion characteristics of corn straw powder, poplar wood chip and rice husk in nitrogen and air, respectively. The Thermogravimetry-Differential Thermogravimetric (TG-DTG) profile shows that the pyrolysis process of these biomass includes three stages of drying, pyrolysis and carbonization, while the combustion process includes three stages of drying, devolatilization and coke combustion. The main reaction stage of biomass pyrolysis and combustion are roughly between 170~400 °C and 180~530 °C, respectively. With the increase of the heating rate, TG and DTG profiles shifts to the high temperature side. Furthermore, the kinetic analysis was performed by using Kissinger-Akahira-Sunose (KAS), Flynn-Wall-Ozawa (FWO), Friedman, and Coats-Redfern (CR) methods, based on the thermogravimetric experimental data. The activation energy of biomass pyrolysis is shown to be between 70~100 kJ/mol. For the activation energy of biomass combustion, the calculated value from isoconversional methods is between 140~180 kJ/mol. The calculated value from CR method is between 80~150 kJ/mol, and the activation energy of the coke combustion stage is greater than that of the devolatilization stage. Finally, the auto-ignition experiment of biomass particles was designed and conducted, indicating that the corn straw powder is more prone to spontaneous combustion, followed by rice husk and poplar wood chip, which corresponds to the results of activation energy. And the fire hazard of the biomass particles was analyzed according to the characteristic parameters. This work provides fundamental data to promote the development of storage techniques and facilitate the safe production of biomass particles.

- **Keywords:** Self-heating; Biomass particle; Combustion; Kinetic analysis; Auto-ignition

Aarthi Kannan, Harikrishnan Venkatesvaran, Dhurkasini Ananthakrishnan, Abinaya Mayavan, Sakthivel Gandhi. *An early detection of prostate cancer drug in water to prevent loss of biodiversity*. Pages 51-62.

Flutamide is a man-made non-steroidal anti-androgen drug that is extensively used for the prostate cancer therapy. Though the drug has a higher benefit ratio in treating cancer, it also exhibits certain lethal side effects to humans. It acts as an environmental pollutant instigating water pollution and aquatic organism damage by interfering in their reproductive cycle and its effect on aquatic life is a major concern. Hence, it is mandatory to detect the presence of this nitro-aromatic compound. For the effective determination of this analyte, gold modified Polyhedral Oligomeric Silsesquioxane (abbreviated as POSS-S-Au) based organic-inorganic hybrid material as chemical modifier has been used. This material synthesized via a hydrolysis-condensation reaction technique followed by a phase transfer method is utilized for the first time in the electrochemical determination of anti-cancer drug. The as-synthesized nanomaterial has been subjected to various Physio-chemical characterization and the Fourier Transform- Infrared Spectroscopy (FT-IR) spectra confirm the presence of -SH organic group and Si-O-Si stretch. X-ray Photoelectron Spectroscopy (XPS) spectra affirms the presence of silicon, oxygen, gold, and Sulphur owing to the introduction of gold through the thiolation of silicate core. The fabricated sensor showed excellent electro-catalytic activity for detecting flutamide with limit of detection (LOD) of 0.12 μM, and higher sensitivity of around 0.048 μA/μM.

- **Keywords:** Anti-androgen drug; electrochemical sensor; environmental pollutant; flutamide; hybrid nanomaterials

Wafa Dastyar, Seyed Mohammad Mirsoleimani Azizi, Mohamed Nouh Ahmed Meshref, Bipro Ranjan Dhar. *Powdered activated carbon amendment in percolate tank enhances high-solids anaerobic digestion of organic fraction of municipal solid waste*. Pages 63-70.

Despite many studies recently investigated the addition of conductive materials for enhancing biomethane recovery in anaerobic digestion, there have been limited efforts to adopt this strategy in high-solids anaerobic digestion (HSAD) with percolate recirculation. In this study, two identical lab-scale mesophilic (36 °C) HSAD systems were operated with the organic fraction of municipal solid waste (OFMSW) under similar operating conditions, including food to microorganism ratio and daily percolate recirculation rate. The percolate tank of the test HSAD system was amended with 15 g/L of powdered activated carbon (PAC). After 30 days of operation, the cumulative biomethane yield for the test reactor was 17 % higher than the control reactor (109 vs. 93 L CH4/kg VS). Furthermore, PAC addition showed additional benefits by lowering free ammonia nitrogen (FAN) and volatile fatty acids (VFAs) concentrations that can inhibit anaerobic digestion. Nonetheless, the preliminary economic analysis suggested that the HSAD amended with PAC is practically challenging and will only be economically feasible if PAC can be recycled and reused for the long-term operation or several cycles.

- **Keywords:** High-solids anaerobic digestion (HSAD); Percolate recirculation; Biomethane; Organic fraction of municipal solid waste (OFMSW); Powdered activated carbon (PAC)

Abbas Mamudu, Faisal Khan, Sohrab Zendehboudi, Sunday Adedigba. *Dynamic risk modeling of complex hydrocarbon production systems*. Pages 71-84.

This study presents a dynamic risk modeling strategy for a hydrocarbon sub-surface production system under a gas lift mechanism. A data-driven probabilistic methodology is employed to conduct a risk analysis. The integrated approach comprises a multilayer perceptron (MLP) – artificial neural network (ANN) model and a Bayesian network (BN) technique. The MLP-ANN model performs the production forecast, and the BN model analyzes dynamic risks (the production response) and evaluates the impact of the sand face pressure on risks. The introduced model offers an effective strategy to avoid

production failure and to monitor dynamic risks. The dynamic risk analysis yields predictive outcomes at any production time in the well's production life. It offers field operators an early warning system based on the Bayesian model with prognostic capabilities. The proposed strategy effectively manages production risks and assists in production decision-making, especially in complex production systems.

- **Keywords:** Bayesian network; Bottom-hole flowing pressure; Dynamic risk; Dual-energy system; Gas lift; Multilayer perceptron

Bing Xiao, Yonggang Li, Bei Sun, Chunhua Yang, Keke Huang, Hongqiu Zhu. *Decentralized PCA modeling based on relevance and redundancy variable selection and its application to large-scale dynamic process monitoring*. Pages 85-100.

In order to ensure the long-term stable operation of a large-scale industrial process, it is necessary to detect and solve the minor abnormal conditions in time. However, the large-scale industrial process contains a large number of complex related process variables, some of which are redundant for abnormal condition detection. To solve this problem, a new decentralized PCA modeling method based on relevance and redundancy variable selection (RRVS-DPCA) is presented. First, considering the complex dynamic relation of process variables, a variable selection strategy based on relevance and redundancy (RRVS) is designed to select variables that carried the most profitable information from different temporal dimensions for each key process variables, so the optimal variable sub-block for each individual key process variables can be obtained. Then, for each sub-block, a corresponding sub-PCA monitoring model is established. The sub-blocks' monitoring results are combined to form a probability statistical indicator through a Bayesian inference. Finally, the weighed contribution plot method is proposed to find the root cause of a fault. The proposed method is compared with several state-of-the-art process monitoring methods on a numerical example and the Tennessee Eastman benchmark process. The comparison results illustrate the feasibility and effectiveness of the proposed monitoring scheme.

- **Keywords:** Decentralized PCA modeling; Bayesian inference; Variable relevance and redundancy; Weighted contribution plot; Large-scale dynamic process monitoring

Oraléou Sangué Djandja, Lin-Xin Yin, Zhi-Cong Wang, Pei-Gao Duan. *From wastewater treatment to resources recovery through hydrothermal treatments of municipal sewage sludge: A critical review*. Pages 101-127.

The treatment of wastewater not only helps to alleviate the scarcity of water and environmental challenges but also generates a by-product called Municipal Sewage Sludge (MSS). The MSS is a high moisture precipitant with plentiful organic and inorganic components. However, some pollutants in MSS components and its high-water content complicate its valorization, and thus, special attention is required for its valorization. Hydrothermal treatments (HTs) can be applied to feedstocks with high moisture content without pre-drying. These processes are gaining more attention to processing MSS into fuels and value-added materials. This work systematically reviews the findings recently emerged from HTs of MSS. The related chemical reactions and the effect of reaction parameters are highlighted based on most recent works. The problems addressed and those not yet addressed are also discussed. Some suggestions are made for the plausible applications of end products with the aim to optimize the whole process. Finally, insight is given into the future of MSS HTs and the concerns that might be the focus of substantial studies.

- **Keywords:** Wastewater; Sewage sludge; Hydrothermal liquefaction; Hydrothermal carbonization; Hydrothermal gasification

G.Y. Bivol, S.V. Golovastov, V.V. Golub. *Effect of channel geometry and porous coverage on flame acceleration in hydrogen–air mixture*. Pages 128-140.

Flame propagation in a hydrogen–air mixture in the presence of porous materials was investigated experimentally in channels with different dimensions and cross–sections. In this study, experiments were performed in a rectangular channel with one or two walls covered with porous material to study flame propagation in stoichiometric hydrogen–air mixtures at room temperature and atmospheric pressure. Depending on the channel configuration, the porous coating of the internal walls ranged from 1/4 to 1/2 of the channel area. Four types of polyurethane foam with a number of pores per inch (PPI) ranging from 10 to 80 were used to cover the channel walls. Flame propagation was visualized using a Schlieren device and high-speed camera. The largest flame acceleration in the porous channel relative to the solid channel was observed in the 20×20mm channel. The ratio of the velocities in the porous channel to the velocity in the solid channels was 6–7 for the porous material with the largest (2.5mm) pores. In the case of a 10×10mm channel, the flame velocity in the porous channel was higher than the flame velocity in the solid channel after 350mm only when using porous coatings with 2.5mm and 1.3mm pores. When using a porous coating with smaller pores the flame velocity was lower than in the solid channel. Schlieren images show different stages of flame propagation from a turbulent flame to a supersonic flame with shock waves.

- **Keywords:** Hydrogen; Porous material; Flame acceleration; Polyurethane foam

Shengchao Rui, Changjian Wang, Shusheng Guo, Rulin Jing, Quan Li. *Hydrogen-air explosion with concentration gradients in a cubic enclosure*. Pages 141-150.

An inhomogeneous hydrogen-air mixture is induced once hydrogen leakage occurs, and an explosion may be triggered due to an accidental ignition with sufficient strength. The effects of different hydrogen concentration gradients on flame behavior and overpressure were experimentally investigated in a closed cubic vessel with a volume of 0.125 m3. The transverse concentration gradients of hydrogen injected from the top face of the vessel were recorded using five oxygen sensors. A high-speed photography was employed to capture the flame shape evolution and the flame tip velocity was derived. Three piezoelectric pressure transducers were mounted on the top and side walls to measure the pressure-time profiles. The results show that the maximum overpressure in homogeneous mixtures is larger than that in inhomogeneous mixtures for fuel-lean hydrogen-air mixtures. However, the maximum overpressure in inhomogeneous mixtures is equal to or larger than that in homogeneous mixtures for fuel-rich hydrogen-air mixtures. Due to a larger difference between the upward and downward flame speeds, a mushroom-like shape flame was recorded in inhomogeneous hydrogen-air mixtures in fuel-lean to slightly fuel-rich hydrogen-air mixtures. The flame speed in two directions has the almost same value in inhomogeneous fuel-richer mixtures. The average flame speed in inhomogeneous mixtures is significantly larger than that in homogeneous mixtures for fuel-rich hydrogen air mixtures.

- **Keywords:** Hydrogen safety; Concentration gradient; Flame shape; Overpressure; Deflagration

Baiwei Lei, Binbin He, Zidong Zhao, Guang Xu, Bing Wu. *A method for identifying the fire status through ventilation systems using tracer gas*

***for improved rescue effectiveness in roadway drivage of coal mines*. Pages 151-157.**

When a coal mine fire occurs, the rescue of trapped mine workers is difficult, because some efficient fire-fighting measures (such as nitrogen injection) cannot be implemented. The development and severity of a fire is difficult to determine, and the integrity of the auxiliary ventilation system may be unknown. These situations pose additional challenges to the trapped mine workers and increase the difficulty level for the rescue team. A novel method using the tracer gas technique is developed to remotely gather information to determine the location and severity of the fire. Laboratory experiments were conducted to understand the tracer gas distribution characteristics when the fire causes damage to the ventilation duct. A mathematical model was developed that uses the tracer gas concentration curve to determine the location and severity of the fire. The model combines the Expectation Maximization (EM) algorithm with the Gaussian Mixture (GM) model. Validated using experimental data, it is demonstrated that the method can determine the fire location with low error. The information collected using this method reflects basic living environmental conditions of the trapped mine workers and provides important input for quickly formulating an effective fire rescue plan that saves lives.

- **Keywords:** Mine fire; Tracer gas; Ventilation; Rescue

Yiming Huang, Jinling Liu, Xinbin Feng, Guojia Hu, Xinyu Li, Leiming Zhang, Lu Yang, Guan Wang, Guangyi Sun, Zhonggen Li. *Fate of thallium during precalciner cement production and the atmospheric emissions*. Pages 158-165.

The cement industry is considered to be an important anthropogenic thallium (Tl) emission source, and yet few reports have been released concerning the fate of Tl during cement production and the emissions of Tl from cement plants (CPs). In this study, three precalciner CPs in the Guizhou province in southwest China were systematically investigated, with all input/output solid materials collected and analyzed. Despite using different raw materials, strong Tl enrichment during the clinker production was observed in all three CPs, with enrichment factors ranging from 85 to 148. Tl concentrations in limestone and most other raw materials were low (0.032–4.163 mg kg−1), but they were 100–700 times higher in the raw meal and kiln tail dust due to circulation and enrichment inside the system. Only a low percentage (3–8 %) of Tl exited the system via the clinker and stack emissions. Atmospheric emission factors of Tl from the three CPs ranged from 0.168 to 0.980 mg Tl tonne−1 clinker, with an average of 0.674 mg Tl tonne−1 clinker. Annual atmospheric Tl emissions from all the CPs were estimated to be 54 kg·yr−1 in Guizhou province and 964 kg·yr−1 over all of China in 2018. Shuttling kiln tail dust may reduce the Tl enrichment during clinker production, and Tl recycled from this material may have commercial value.

- **Keywords:** Thallium; Precalciner cement plants; Enrichment factors; Atmospheric emissions

Jitao Cai, Jiansong Wu, Shuaiqi Yuan, Zhe Liu, Desheng Kong. *Numerical analysis of multi-factors effects on the leakage and gas diffusion of gas drainage pipeline in underground coal mines*. Pages 166-181.

Gas drainage system is a critical technique to prevent gas outbursts in the underground coal mine. The leakage of gas drainage pipelines can pose serious threats to the safety production of underground mining. In this paper, a multi-factors gas drainage pipeline leakage and diffusion (GDPLD) model is proposed based on the OpenFOAM platform, which can analyze the leakage and diffusion characteristics inside the pipelines. With field measurement data in a coal mine, the GDPLD model is verified with good practicability.

Furthermore, scenario analysis in the context of different leak sizes, locations, and pipeline diameters is presented to evaluate the specific characteristics of gas leakage and diffusion inside the pipeline with negative pressure. The results showed that the leakage accident close to the pump station with a large leak size and small pipeline diameter usually represents the worst case, and when gas sensors are installed downstream of the leakage location, it is helpful to realize effective detection of the leakage accident. This study can help to improve the understanding of the leakage and diffusion characteristics of gas drainage pipelines and provide technical supports for the monitoring system design of the gas drainage pipelines in underground coal mines.

- **Keywords:** Underground coal mine; Gas drainage pipelines; Gas leakage and diffusion; Computational fluid dynamics; OpenFOAM

Mahoko Ando, Michiya Fujita, Yu-ichiro Izato, Atsumi Miyake. *A kinetic model for the autocatalytic behavior of nitric acid/formic acid mixtures to predict induction period*. Pages 182-187.

Prevention of runaway reactions is one of the ultimate goals of process safety engineering. However, the lack of knowledge for mechanism and kinetics of autocatalytic reactions enables to design safer processes handling reactive materials. The purpose of the present study was to accurately predict the induction period of autocatalytic reaction system composed by nitric acid and formic acid using a sophisticated kinetic model for the autocatalytic behavior. The reactions of nitric acid with organic compounds are autocatalytic and so can rapidly generate large amounts of heat and pressure without obvious warning signs. Thermal analyses were carried out using a reaction calorimeter while ion chromatography was employed to quantify reaction products. Exothermic reactions were observed to begin when the concentration of nitrous acid, which was identified as the autocatalyst, exceeded 4.6 ± 1.2 mmol L−1. A kinetic model was determined as d[HONO]/dt = 2.62 × 1012exp(1.06 × 104/T)·[HNO3]2.5±0.1[HCOOH]1.8±0.1[HONO]1.9±0.1. This model was in good agreement with other results obtained from reaction calorimetry.

- **Keywords:** Autocatalytic reaction; Kinetic model; Induction period; Nitric acid; Formic acid

Meral Yurtsever. *Are nonwoven fabrics used in foods made of cellulose or plastic? Cellulose/plastic separation by using Schweizer's reagent and analysis based on a sample of tea bags*. Pages 188-194.

Tea ranks high among the most popular drinks worldwide, second only to water. But the term covers a very wide range of products, extending from common black tea to herbal teas containing elements of various plant species, offered in bulk tea as well as tea bag form. Tea bags are a popular option worldwide, given the ease of use they offer. It is often noted that tea bags are made of cellulose, save for some exceptions made completely of nylon or PET plastics (silken, pyramid). The present study is essentially an analysis of tea bags occupying a significant portion of the shelf space in the tea section of supermarkets, which are purportedly made of cellulose. In this context, Schweizer's reagent (SR), a strong solvent of cellulose, was applied within the framework of ATR-FT-IR analyses to see whether any plastics were used in the nonwoven fabric of cellulose tea bags. The analysis of various brands of tea bags purchased from various supermarkets in Turkey revealed that 4 out of 11 tea bags for use in teacups, called cellulose bags, contained plastics (polyester, PE, and PP-PE blends), whereas the figure for the tea bags for use in the teapot was 11 out of 11. Whenever tea bags are used in brewing hot drinks such as tea, often consumed for its enjoyable taste and as a herbal remedy, the bag may contain plastic fibers, posing potential health risks. Furthermore, the use of durable

materials such as plastics in tea bags, which are purportedly compostable products, also constitutes a risk in terms of environmental sustainability.

- **Keywords:** Cellulose teabag; Filler material; Polymer; Schweizer's reagent (SR); Stakeholder; Sustainability

Yuri Abner Rocha Lebron, Victor Rezende Moreira, Priscila Barbosa Moser, Lucilaine Valéria de Souza Santos, Miriam Cristina Santos Amaral. *Screening cost effectiveness and salinity build up control in osmotic membrane bioreactors for refinery wastewater treatment: A draw solute with lower diffusivity and ultrafiltration implementation*. Pages 195-207.

Two strategies were investigated for salinity build up prevention in osmotic membrane bioreactors (OMBR) treating a real refinery wastewater. Firstly, a solute with lower diffusivity (MgCl2, for 102 days) was used. The impact on the microbiological activity was lower, which favored the recalcitrant compounds degradation. However, without salinity relief, the mixed liquor (ML) salinity increased, impacting the forward osmosis (FO) flux (0.18 L/m2h). Secondly, an ultrafiltration (UF) membrane was submerged within the ML and the draw solution (DS) replaced to NaCl. The ML conductivity was stable along 330 days without a severe flux decay (1.07 L/m2h). Nonetheless, the reverse NaCl flux had a higher impact on the microbiological activity and the concentration of dissolved organic carbon and ammoniacal nitrogen started to increase in the UF permeate. Due to the lower permeate flux, the OMBR had a higher membrane area requirement which represented the main contributor for the total operating costs.

- **Keywords:** Salinity build up; OMBR; Wastewater treatment; Draw solution; Hybrid UF-OMBR; Recalcitrant compounds

Chunxiang Liu, Mehdi Jangi, Jie Ji, Longxing Yu, Long Ding. *Experimental and numerical study of the effects of ullage height on plume flow and combustion characteristics of pool fires*. Pages 208-221.

Pool fires are frequently reported to trigger domino effects in oil storage farms and chemical factories. Fire plume is the vehicle of damage caused by pool fires. This study aims to study the effects of ullage height (distance between the fuel surface and the upper pool rim) on fire plume flow and combustion characteristics were conducted by experimental and numerical studies. Ullage heights were systematically changed from zero to the value at which the flame is self-extinguished. Simulations were validated against both time-averaged and instantaneous experimental measurements. In terms of the dynamic of the flame base with respect to the pool outlet, three classes were identified as follows. Class I: Flame base anchored near the upper pool rim, and the combustion was mainly of classic non-premixed flame type; Class II: Flame base entered into the pool but not merged; Class III: Flame base entered into the pool and merged along the middle axis. It was shown that the decreasing pressure near the pool outlet driven the flame to enter into the pool, as ullage height increased. According to the time-history of plume flow, three plume flow patterns were revealed at different ullage height conditions, which explained the evolutions of flame structures. It was shown that the percentage of premixing combustion was increased with ullage height. This behavior was attributed to the enhanced fresh air entrainment and mixing at the flame base.

- **Keywords:** LES; Plume flow; Combustion mode; Ullage height; Flame characteristics; Pool fire

Bahram Ghorbani, Armin Ebrahimi, Masoud Ziabasharhagh. *Thermodynamic and economic evaluation of biomethane and carbon*

***dioxide liquefaction process in a hybridized system of biogas upgrading process and mixed fluid cascade liquefaction cycle*. Pages 222-243.**

In recent years, the use of liquefied biogas in the power plant for peak shaving and transportation industries from an environmental and economic perspective has been considered. Simultaneous design of biogas purification and liquefaction processes reduces the number of equipment required and energy consumption. In this paper, a novel purification and liquefaction integrated structure includes a biogas upgrading process by cryogenic separation and amine scrubbing methods and a biomethane liquefaction cycle based on the mixed fluid cascade. In this integrated structure, 2.393 kg/s biogas and 2730 kW power are consumed and 0.5387 kg/s bioLNG, 0.1280 kg/s bioCH4, and 0.2102 kg/s liquid bioCO2 are produced along with 1.625 kg/s hot water. The required cooling of cryogenic biogas upgrading and required heat for the biogas upgrading by amine scrubbing method are provided through mixed refrigerant cascade cycles and waste heat in the integrated structure, respectively. The total thermal energy and exergy efficiencies are 73.11 % and 72.58 %, respectively. The specific power consumption and coefficient of performance of the mixed fluid cascade cycle are calculated to be 0.4761 kW h/kg bioLNG and 3.675, respectively. The economic analysis illustrates that the prime cost of product and return period are 0.2399 US$/kg LNG and 2.122 years, respectively.

- **Keywords:** Process integration; Biogas upgrading process; Mixed fluid cascade liquefaction cycle; Liquified biomethane; Liquid bioCO2; Economic and exergy analyses

Fatemeh Aghili, Ali Asghar Ghoreyshi, Bart Van der Bruggen, Ahmad Rahimpour. *A highly permeable UiO-66-NH2/polyethyleneimine thin-film nanocomposite membrane for recovery of valuable metal ions from brackish water*. Pages 244-256.

A positively charged thin film nanocomposite (TFN) membrane was synthetized based on the nano-gel UiO-66-NH2 for fractionation of monovalent and multivalent ions from saline water. The addition of nano-gel UiO-66-NH2 in the aqueous phase containing polyethyleneimine (PEI) led to the fabrication of a nanofiltration (NF) membrane with a looser structure, which can enhance the water permeability. The resulting TFN/PEI membranes were found to have a high rejection of 97.4 % and 88.1 % to MgCl2 and MgSO4 and a very low rejection of 4.1 % and 6.1 % for LiCl and NaCl with a permeability above 38 L/m2.h.bar. The TFN/PEI-3 membrane with 1 wt% nano-gel UiO-66-NH2 in PA layer had an optimal selectivity and permeability for fractionation of Mg2+/Li+ in MgCl2/ LiCl solution and Mg2+/Na+ in MgSO4/ NaCl solution. An efficient separation of Mg2+/Li+ with separation factor of 33, accompanied by a permeability as high as 30.6 L/m2.h.bar, was obtained. Moreover, the high hydrophilicity of the UiO-66-NH2-based TFN/PEI membrane led to a reasonable value of 82.6 % flux recovery after three cycles of filtration of a 2000 ppm Mg2+/Li+ mixed solution. These results demonstrate that this UiO-66-NH2-based TFN/PEI membrane with high permeability and selectivity can be an appropriate candidate for lithium extraction in practice.

- **Keywords:** UiO-66-NH2; Thin film nanocomposite (TFN); Positively charged membrane; Mono/divalent ions separation; Lithium extraction

Khairul Anwar Mohamad Said, Ahmad Fauzi Ismail, Zulhairun Abdul Karim, Mohd Sohaimi Abdullah, Asif Hafeez. *A review of technologies for the phenolic compounds recovery and phenol removal from wastewater*. Pages 257-289.

The immoderate amount of phenol found in the water reservoir, i.e., river and municipal drain, has served as one major contributor to the scarcity of potable water worldwide.

Many conventional methods have been applied to tackle polluted phenol water but suffer from various drawbacks. Special attention has been given to the photocatalytic membrane due to its ability to degrade phenol and sieving, a 2-in-1 function. Hence, this extensive report reviewed the extant trends in phenol removal such as distillation, adsorption, biodegradation, chemical oxidation, electrochemical oxidation, enzymatic treatment, and membrane technology. The in-depth discussion concerning the utilization of membrane as photocatalyst support media is also conferred, which could be the trendsetter in several years to come.

- **Keywords:** Conventional phenol treatment; Membrane technology; Phenol photodegradation; Photocatalyst; Photocatalytic membrane

Yasin Orooji, Mohammad Javadi, Hassan Karimi-Maleh, Alireza Zamani Aghaie, Kazem Shayan, Afsaneh L. Sanati, Rozhin Darabi. *Numerical and experimental investigation of natural gas injection effects on NOx reburning at the rotary cement kiln exhaust*. Pages 290-298.

Thermal NOx formation is very high in the rotary cement kiln due to high-temperature flame. Essentially all NOx emissions associated to the cement manufacturing are formed in cement kilns. In this paper, the effects of natural gas injection into calciner exhaust, i.e., rotary kiln inlet, on NOx reburning by CO and CH radicals is numerically and experimentally investigated. A 3D model of turbulent combustion flow to stimulate the NOX reburning on an industrial scale is developed by the finite volume method. The results show that the NOx reduction can be reached 30 % and 70 % by 950 m3/h and 2750 m3/h natural gas injection, respectively. Furthermore, by increasing natural gas injection flow rate and reaction time, NOx reduction rate is abruptly decreased. The experimental results imply 65 % NOx reduction by natural gas injection from walls of rotary furnace channel inlet where good agreement by numerical results is well proved. Obtaining results also prove that the NOx return in swirling region is highly increased and NOx concentration remarkably reduced.

- **Keywords:** Cement kiln; NOx reburning; Methane injection; Calciner; Numerical simulation

Kai Wang, Xiang Zhang, Liang Wang, Lei Li, Meng Zhang, Aitao Zhou. *Experimental study on propagation law of shock wave and airflow induced by coal and gas outburst in mine ventilation network*. Pages 299-310.

Coal and gas outburst seriously threatens the safety of underground coal mining. After the outburst, it will not only cause harm in the near-field outburst roadway but may also have a strong impact on the far-field ventilation network connected to the outburst roadway, expanding the impact of the disaster. In order to define the propagation law of shock wave and airflow induced by the outburst and its influence on the far-field ventilation network, the coal and gas outburst experimental system was used to carry out an experimental study under different air current and local resistance conditions in this paper. The results show that, under different air current states, the first overpressure peak increases with an increase of outburst pressure and decreases with an increase of propagation distance. Compared with the propagation characteristics in a windless roadway, the first overpressure peak and attenuation coefficient of shock wave propagating downwind are smaller, whereas opposite in upwind state. The local resistance enhances the impact and disturbance ahead of it and weakens that after it. When shock airflow propagates downwind, the increase of shock airflow velocity is approximately equal to the original airflow velocity in the roadway, whereas the airflow direction may reverse when the shock airflow propagates upwind. This paper provides some references to prevent the impact expansion of coal and gas outburst, which are of

great significance for the optimization of ventilation network and emergency management.

- **Keywords:** Coal and gas outburst; Shock wave attenuation; Airflow disturbance; Far-field ventilation network

Zhaojin Lu, Xiaoyong Yang, Bingjie Wang, Hui Li, Zhishan Bai. *Coalescence-adsorption coupling treatment instead of alkaline washing-water washing process for efficient removal of sulfuric acid and sulfates*. Pages 311-323.

C4 alkylate oil is an ideal blending component of automotive gasoline, and the green removal of sulfuric acid and sulfates from the high-temperature sulfuric acid alkylation reaction products (SAARP) has always been a hot issue in the field of clean alkylation production. In this paper, a novel coalescence separation-depth adsorption (CS-DA) coupling dry separation technique is introduced to efficiently separate acid-hydrocarbon emulsions, with the aim to supersede the alkaline washing-water washing (AW-WW) process in alkylation unit. Lateral line tests were conducted on the coupling treatment of the alkylation reaction products (ARP) produced in the STRATCO alkylation unit of Sinopec Tianjin Branch. The sulfur morphology analysis shows that the sulfides in the ARP mainly come from C4 feedstocks and alkylation reaction, including mercaptans, thioethers, thiophenes, trace hydrogen sulfide and sulfur dioxide. The mechanism of coalescence separation reveals that the efficient removal process of sulfuric acid by fiber coalescence separation also has a function similar to "pickling extraction" to remove sulfates. In addition, we investigated the influence of CS-DA coupling treatment on the total sulfur and sulfuric acid content in the ARP and performed the copper corrosion and water-soluble acid assays. The research findings indicated that the back sideline of the acid coalescer had the most outstanding separation effect relative to the front and rear lateral lines of the heat exchanger. The total sulfur content in the ARP after separation can be reduced to less than 5 mg/L, without water-soluble acid and copper corrosion (1a). The industrial application shows that the CS-DA coupling dry separation technique can completely replace the AW-WW process, which makes the various indicators of alkylate oil strictly controlled and the sulfur content up to the industrial standard. The novel dry separation technique provides a promising alternative for solving the difficulties in the emulsion treatment of high-temperature sulfuric acid alkylation and promoting the clean production of alkylation.

- **Keywords:** Sulfuric acid alkylation; Acid-hydrocarbon emulsion; Fiber coalescence; Deep adsorption; Alkaline water washing cancellation

Muhammad Izhar Shah, Muhammad Faisal Javed, Abdulaziz Alqahtani, Ali Aldrees. *Environmental assessment based surface water quality prediction using hyper-parameter optimized machine learning models based on consistent big data*. Pages 324-340.

Prediction of dissolved oxygen (DO) and total dissolved solids (TDS) are of paramount importance for water environmental protection and analysis of the ecosystem. The traditional methods for water quality prediction are suffering from unadjusted hyper-parameters. To effectively solve the hyper-parameter setting problem, the present study proposes a framework for tuning the hyper-parameters of feed forward neural network (FFNN) and gene expression programming (GEP) with particle swarm optimization (PSO). Thereafter, the PSO coupled hybrid feed forward neural network (PSO-FFNN) and hybrid gene expression programming (PSO-GEP) were used to predict DO and TDS levels in the upper Indus River. Based on thirty years consistent dataset, the most influential input parameters for DO and TDS prediction were determined using principal component analysis (PCA). The impact on the model performance was evaluated employing five

statistical evaluation techniques. Modeling results indicated excellent searching efficiency of the PSO algorithm in optimizing the structure and hyper-parameters of the FFNN and GEP. Results of PCA revealed that magnesium, chloride, sulphate, bicarbonates, specific conductivity, and water temperature are appropriate inputs for DO modeling, whereas; calcium, magnesium, sodium, chloride, bicarbonates and specific conductivity remained the influential parameters for TDS. Both the proposed hybrid models showed better accuracy in predicting DO and TDS, however, the hybrid PSO-GEP model achieves better accuracy than the PSO-FFNN with R value above 0.85, the root mean squared error (RMSE) below 3 mg/l and performance index value close to 1. The external validation criteria confirmed the resolved overfitting issue and generalized results of the models. Cross-validation of the model output attained the best statistical metrics i.e. ($R = 0.87$, $RMSE = 2.67$) and ($R = 0.895$, $RMSE = 2.21$) for PSO-FFNN and PSO-GEP model, respectively. The research findings demonstrated that the implementation of artificial intelligence models with optimization routine can lead to optimized models for accurate prediction of water quality.

- **Keywords:** River water quality; Environmental protection; Machine learning modeling; Particle swarm optimization; Principal component analysis; Cross-validation

Atefeh Esfandiari, Dariush Mowla. *Investigation of microplastic removal from greywater by coagulation and dissolved air flotation*. Pages 341-354.

Microplastics (MPs) have recently become a controversial issue, mainly due to their eco-toxicological effects on aquatic environments. Although a typical wastewater treatment plant (WWTP) removes a large number of MPs from the wastewaters, final effluents are yet considered to be the primary sources of MP contaminations into the environment. Hence, there should be a tertiary treatment called advanced wastewater treatment technology for efficient MP removal. In the current research, Al-based and Fe-based coagulants were used in a dissolved air flotation (DAF) cell as an advanced wastewater treatment technology to remove polyethylene (PE) MPs from greywater, which is one of the most predominant types of MPs found in the greywater. PE reduction up to 96.10 % and 70.56 % were observed for Al- and Fe-based coagulants, respectively. The operative parameters, including pressure, pH, coagulant dosage, and water flow rate into the flotation cell, were identified. The experimental design was developed using Design-Expert software to investigate and maximize the PE removal efficiency. As a result, some sufficiently accurate statistical models were proposed to obtain the optimum quantities of the respective factors. It was determined that the most effective removal was achieved with 5.95 bar saturation pressure, pH 6, 14.46 mg/L coagulant concentration, and 680.5 mL/min water flow rate into the flotation cell using AlCl3·6H2O as the coagulant.

- **Keywords:** Advanced wastewater treatment technology; Coagulant; Design-Expert; Dissolved air flotation; Greywater; Polyethylene microplastic

Sheng Shang, Mingshu Bi, Tianjiao Zhang, Haipeng Jiang, Shulin Zhang, Wei Gao. *Synthesis of green nanomaterial and discussion on its suppression performance and mechanism to aluminum dust explosion*. Pages 355-364.

In order to develop a green and efficient nano suppressant for aluminum (Al) dust explosion, MCN with layered structure was synthesized with low-cost urea as precursor via simple calcination technology. The suppression performance of MCN on the flame propagation of 30 μm and 5 μm Al dust with the concentration of 1000 g/m3 was experimentally studied. Results showed that with the addition of MCN increasing, the flame luminous intensity, flame propagation velocity and fluctuating trend of mixture-Al

dust were greatly decreased. After adding 500 g/m3 and 700 g/m3 to 30 μm and 5 μm Al dust, the average flame propagation velocities declined by 73.24 % and 94.07 % separately. The minimum inerting concentration of 30 μm and 5 μm Al dust was 600 g/m3 and 900 g/m3. Explosion residuals were analyzed to further reveal the suppression mechanism of MCN in detail. The good performance of MCN provided a potential direction to develop efficient suppressants on the suppression of Al dust explosions to improve process safety.

- **Keywords:** Aluminum dust explosion; Nano suppressant; Flame propagation behaviors; Suppression mechanism

Dooguen Song, Kwangho Lee, Chuntak Phark, Seungho Jung. *Spatiotemporal and layout-adaptive prediction of leak gas dispersion by encoding-prediction neural network*. Pages 365-372.

Gas leak accident has been troublesome issues in the chemical industries. Predicting dispersion boundaries are important to make rapid and proper actions. Currently, computational fluid dynamics (CFD) are used to predict the dispersion boundaries. However, when the facility-layout of a workplace is often modified, using CFD is not desirable since it requires large computational expenses. This study proposes an encoding-prediction neural network to learn representations between dispersion of leak gas, velocity field, and facility-layouts. This network predict volume fraction field of leak gas in $t + k\Delta t$ timestep by observing that data in $t \sim t + (k-1)\Delta t$ timestep. Training and test losses are decreased to $1.04 \times 10{-}5$ and $1.46 \times 10{-}5$, respectively. The network predicts dispersion of leak gas through recursive prediction scheme, the predicted results shows good agreement with ground truth. Methodology to generated various facility-layouts, and preprocessing methods to deal with skewed data are suggested. The methodology and results proposed in this study would be useful for developing the CFD surrogate model.

- **Keywords:** Gas leak; Dispersion; Spatiotemporal; Layout-adaptive; Neural network

Jarosław Brodny, Magdalena Tutak. *Applying computational fluid dynamics in research on ventilation safety during underground hard coal mining: A systematic literature review*. Pages 373-400.

The safety of the coal production process, which in the coming years will continue to be one of the basic energy resources in many countries worldwide, has a significant impact on its efficiency. The random character of many hazardous phenomena accompanying this process requires the application of both modern and safe methods to study these phenomena. Model studies based on the Computational Fluid Dynamics (CFD) method are known to have such features. They enable the analysis of very complex and hazardous phenomena, which are hard or even impossible to investigate with the use of other methods. Therefore, this article focuses on the analysis of the state of the art in terms of the Computational Fluid Dynamics application in research on ventilation safety during underground hard coal mining. It was assumed that CFD-based studies may significantly improve the safety of the mining production process. For this purpose, a systematic literature review was carried out, which – according to the adopted methodology – involved four research questions. The review included scientific publications (articles) contained in the two most prestigious databases, i.e., the Web of Science and the Scopus. In accordance with the adopted search criteria, articles that used the Computational Fluid Dynamics method and focused on ventilation safety during underground coal mining were selected. The meta-analysis of these data made it possible to identify seven thematic areas undertaken in these publications. The following paper presents a list of articles assigned to these groups with selected items being discussed. On the basis of the conducted research, comprehensive answers to the research

questions were provided. The results systematize the knowledge of CFD application in research on ventilation safety in mining. Also, they are a valuable source of information for future researchers and engineers concerned with the safety of the mining production process. Moreover, potential directions of further research in the field of possible Computational Fluid Dynamics applications were indicated to improve the safety of the process in question.

- **Keywords:** Computational fluid dynamics; Mining production process; Ventilation hazards; Safety; Systematic literature review

Thanapha Numpilai, Chin Kui Cheng, Jumras Limtrakul, Thongthai Witoon. *Recent advances in light olefins production from catalytic hydrogenation of carbon dioxide*. Pages 401-427.

Increasing concerns of global warming problems caused by rising CO2 concentration in the atmosphere have driven many activities and researches for the reduction of CO2 emission. A huge CO2 emission has been discharged from industrial sectors arising from materials processing. Therefore, the development of efficient processes for the reduction of CO2 emission in the industry sector is vital. One of promising ways is to utilize CO2 as a carbon source for the production of high value-added chemicals including light olefins. In order to make the CO2-to-light olefin process feasibility in terms of economic point of view, efficient catalysts are essential for maximizing selectivity and yield of light olefins. This review summarizes recent progresses in rational design of catalytic system for CO2 conversion to light olefins. Two different paths for CO2 hydrogenation to light olefins, including the CO2−Fischer−Tropsch (CO2-FT) and oxygenate-mediated (like methanol, dimethyl ether, etc.), are compared in terms of catalytic performance and C2–C4 olefins productivity. In the CO2-FT route, the selective production of the desired C2–C4 olefins is the key goal of development with an emphasis on synergy control between active metals, promoters and supports for tuning the surface H/C ratio which significant relevance to the C2–C4 olefins formation. While, an improvement in activity with suppressing secondary reaction is imperative for achieving a high C2–C4 olefins productivity in oxygenate-mediated. Besides optimizing the catalyst components (i.e., metal oxide/zeolite mass ratios and zeolite acidity) as well as operating conditions, the distance control of the two active components is another crucial to reach the satisfactory performance. Recently, a novel catalytic system using multifunctional catalysts composed of In2O3/SAPO-34 and Fe-Co/K-Al2O3 catalysts provides an unprecedented high C2–C4 olefins productivity, shedding light on the prospects for economic competitiveness and growth in the market economy.

- **Keywords:** CO2 hydrogenation; Light olefins; CO2−Fischer−Tropsch route; Oxygenate-mediated route