Process Safety and Environmental Protection

Rok 2022, Volume 161

May

Meilin Liu, Yangpeng Liu, Huazhong Sun, Jian Hu, Xishi Wang. *Experimental study on the interaction of water mist spray with two buoyant non-premixed flames*. Pages 1-12.

Single-fire and double-fire extinguishments by water mist were conducted to assess the similarities and differences. The double-fire extinguishment requires higher applied volume flux of the water mist and spray momentum, while it is achieved faster than the single-fire extinguishment, owing to the smaller size of the single flames of the double-fire. Both the air entrainment restriction among the two flames of the double-fire and the typical re-ignition phenomenon have a significant effect on the double-fire extinguishment. A double-fire merging from the burner surface is more difficult to be extinguished in terms of the critical operating pressure since the air entrainment restriction among the two flames of the double-fire is more intense. A double-fire with a smaller flame spacing requires a longer extinguishing time since re-ignition happens more easily. The equivalent diameter (De) is applied to calculate the plume–spray thrust ratio of the double-fire and evaluate the competition between the double-fire and the water mist quantitatively.

- **Keywords:** Water mist; Double-fire extinguishment; Process safety; Equivalent diameter; Plume–spray thrust ratio

Fei Xiao, Hongxia Zhang, Tianzhao Wu, Jiahao Liu, Jianxin Liu, Jiangbo Zhang, Wei Liu, Taixin Liang, Jinghui Hu. *Superhydrophobic/superlipophilic interface layer for oil-water separation*. Pages 13-21.

Low-cost, stable materials that can be used for oil-water separation have significant industrial applications. A simple two-step immersion approach was used to successfully create a melamine sponge with superhydrophobic/superlipophilic characteristics. The polyphenolamine@ 1 H,1 H,2 H,2 H-perfluorodecyltrichlorosilane sponge (PPA@PF sponge) produced in this study possesses exceptional superhydrophobic and superlipophilic properties. Scanning electron microscopy (SEM), infrared spectroscopy (IR), and X-ray photoelectron spectroscopy (XPS) were used to examine the surface morphology and chemical content of the PPA@PF sponge. The prepared PPA@PF sponge has a static contact angle (SCA) of 156°. More notably, PPA@PF sponge has extremely stable and anti-corrosion properties. After being corroded by acidic solutions, alkaline solutions, and organic solvents, the PPA@PF sponge retains good hydrophobic

characteristics on its surface. Finally, the PPA@PF sponge is successfully applied to the rapid oil-water separation.

- **Keywords:** Superhydrophobic; Superlipophilic; Melamine sponge; Polyphenolamine; Oil-water separation

Zhongqi He, Yuntian Qu, Wenbiao Jin, Xu Zhou, Wei Han, Kang Song, Shuhong Gao, Yidi Chen, Shiyu Yin, Guangming Jiang. *Effect of microwave on biomass growth and oxygen production of microalgae Chlorella pyrenoidosa cultured in real wastewater*. Pages 22-33.

The oxygen production efficiency of microalgae is a critical factor for the performance of algal-bacterial symbiotic systems during real wastewater treatment. This study proposed a new method to enhance the growth and oxygen production rate of microalgae via microwave irradiation. The oxygen production performance of Chlorella pyrenoidosa grown in real wastewater was evaluated in the presence of microwaves, and the photosynthetic oxygen production rate was calculated based on the produced chlorophyll-a and dissolved oxygen. The results showed that microwave treatment promoted both algal growth and oxygen production. Chlorella pyrenoidosa was irradiated by microwave during the logarithmic phase. When the radiation power was 400 W and the treatment time was 25 s, the oxygen production of Chlorella pyrenoidosa and chlorophyll-a increased by 10.7% and 12.4%, while the photosynthetic oxygen production rate increased by 5.8%. Therefore, microwave can save the aeration energy required for degrading organic matter in real wastewater by algal-bacterial systems.

- **Keywords:** Microwave; Chlorella pyrenoidosa; Real wastewater; Photosynthetic oxygen production rate; Algal-bacterial symbiotic

Mohd Amirul Mukmin Abdullah, Mazrul Nizam Abu Seman, Syed Mohd Saufi Tuan Chik, Syamsul B. Abdullah. *Factorial design in optimizing parameters for thermoresponsive ionic liquids as draw solution*. Pages 34-49.

This study aims to optimize the operating conditions of the forward osmosis (FO) process by introducing thermo-responsive ionic liquids (TRILs) namely 1-butyl-3-methylimidazolium tetrafluoroborate ([Bmim][BF4]) as a draw solution for seawater desalination applications. The influence of the operation parameters, such as the feed and draw flowrate (60–300 ml/min), draw solution concentration (0.6–3.0 M), temperature (25–50 °C), and type of flow with feed concentration using artificial seawater (0.6 M NaCl). The interaction between parameters has been specified using fractional factorial design (FrFD). The draw solution concentration and the interactions between draw and feed flowrate were the most significant factors in achieving high water flux 5.1 LMH. Besides that, the draw flowrate and the interaction of both draw and feed flowrate give high significance toward adverse effects (such as concentration polarization), which is good to obtain low reverse salt at 1.3 gMH. Use the desirability function (DF) to obtain the highest water flux of 5.04 LMH and the lowest reverse salt flux of 1.71 gMH, with a desirability of 0.95. The optimal condition for FO performance is 300 ml/min feed and draw flowrate with 3.0 M draw solution at 25 °C and co-current flow.

- **Keywords:** Forward osmosis; Desalination; Factorial design; Optimal condition; Ionic liquids; Draw solution

Fengbin Zhao, Rongxing Bian, Tingxue Zhang, Xin Fang, Xiaoli Chai, Mingxue Xin, Weihua Li, Yingjie Sun, Liqun Yuan, Jian Chen, Xuan Lin, Lili Liu. *Characteristics of polychlorinated dibenzodioxins/dibenzofurans from a full-scale municipal solid waste (MSW) incinerator in China by MSW classification*. Pages 50-57.

The physical and chemical compositions of municipal solid waste (MSW) are important factors affecting the formation and release of polychlorinated dibenzodioxins/dibenzofurans (PCDD/Fs). A 4-year investigation (2017–2020) of the emission characteristics of PCDD/Fs from the flue gas and fly ash by a full-scale MSW incinerator in Ningbo city, Zhejiang province was conducted. This was undertaken to determine the implications of sorting MSW. Results showed that progress made in classifying MSW has led to a significant decrease in the proportion of kitchen waste components, the moisture and chlorine contents of MSW. However, there has also been a significant increase in the proportion of textile and wood components and calorific value. Approximately 60% of the PCDD/Fs generated during MSW incineration were captured in the fly ash that enters the filter bag. The PCDD/Fs emission factors were significantly positively correlated with the proportion of kitchen waste, plastics and heavy metal elements Fe, Ni, Mn, Cr, Pb, Cd, and Zn in the MSW, and negatively correlated with the wet-based high and low calorific values of the MSW. A decreasing trend in PCDD/Fs generation and emission from 3339.3 ng/t MSW in 2018–1787.5 ng/t MSW in 2020 was observed since the implementation of MSW classification as it can reduce the quantity of kitchen waste and plastics, and improve the calorific value of the MSW.

- **Keywords:** Municipal solid waste classification; Waste incineration; Polychlorinated dibenzodioxins; Polychlorinated dibenzofurans; Fly ash

Won-Taek Hong, Jong-Sub Lee, Dongsoo Lee, Hyung-Koo Yoon. *Estimation of bulk electrical conductivity in saline medium with contaminated lead solution through TDR coupled with machine learning*. Pages 58-66.

Time-domain reflectometry (TDR) has been used for the characterization of media; however, the results of TDR tests significantly differ according to the types of solutions. The objective of this study is to suggest a new relationship between TDR output values and bulk electrical conductivity based on a machine learning algorithm for enhancing the reliability of TDR measurement. Various salinities (0%, 1%, 2%, and 3%) and lead concentrations (0, 0.5, 1, 2, 5, and 10 mg/L) are applied along with silica sand, classified as SP in USCS, to create media. A laboratory test is performed to measure the TDR waveform at the bottom of the cylindrical cell, and a resistance probe is also installed to obtain the true bulk electrical conductivity in the cell. A deep neural network machine learning algorithm is applied to establish the relationship between the TDR output value and the bulk electrical conductivity at each frequency of 0.1, 0.12, 1, 10, and 100 kHz. The highly important variables are also defined through random forest. This study demonstrates that the TDR can be reliably converted into bulk electrical conductivity when two different solutions are mixed.

- **Keywords:** Bulk electrical conductivity; Lead solution; Deep neural network; Salinity; Time-domain reflectometry (TDR)

Muhammad Saqib Nawaz, Talal Alamoudi, Sofiane Soukane, M. Obaid, Noreddine Ghaffour. *Effect of colder stream temperature control on energy utilization, flux, RSF, and membrane integrity in asymmetric temperature FO systems*. Pages 67-77.

Water and energy are key components to assess the feasibility of any water treatment technique. For industrial applications of forward osmosis (FO), energy optimization needs to be explored further. Asymmetric temperature conditions, having different feed solution (FS) and draw solution (DS) temperatures, are likely to occur in industrial FO applications and are least explored. Some standard practices are followed without any scientific evidence of their impact on the system performance and energy utilization, like maintaining the colder stream temperature instead of letting it reach a steady state with the hotter stream. This study compares water flux, reverse solute flux (RSF), and energy utilization when the colder stream temperature is maintained and not maintained. Thin film composite-poly amide (TFC-PA) and cellulose triacetate (CTA) membranes were used at laboratory-scale in 24 h batch experiments with 0.75 M NaCl as DS and DI water as FS. All possible configurations of membrane orientation (AL-DS and AL-FS) and streams heating and cooling strategies were studied. The module material was made up of plexi-glass with 4 cm thick plates and flexible tubing of PVC was used. Results revealed that under not maintained conditions, on average, the water flux increased by 9.1–17%, RSF increased by 13.8–27.3%, and energy consumption reduced by 75.8–67% with CTA and TFC membranes, respectively. Therefore, if the RSF is not the primary concern of the application, it is advantageous not to maintain the colder stream temperature. However, it is recommended that scientists verify and compare the efficiencies between maintained and not maintained temperatures under their specific experimental conditions.

- **Keywords:** Water-energy nexus; Asymmetric temperature; Forward osmosis; Energy optimization; Reverse solute flux

Guoqing Xiao, Shuo Wang, Hongfu Mi, Faisal Khan. *Analysis of obstacle shape on gas explosion characteristics*. Pages 78-87.

The safe design and operation of clean fuels like hydrogen require a detailed understanding of their explosion characteristics. An experimental study of the flame propagation behavior influenced by quadrangular, cylindrical, and triangular obstacles was executed in a 530 mm × 82 mm × 82 mm pipe. The results confirm the understanding that obstacles with a tip promote the generation of flow instability and produce a more intense burning behavior of the flame. The shear layers shed fewer larger vortices after the quadrangular obstacle; however, these vortices can be dislodged to form smaller and more vortices after passing through the triangular obstacles. The shear layer has weak shedding properties behind obstacles with curved edges. In the flame propagation process, the quadrangular obstacles have a more obvious promoting effect of the initial explosion, but the degree is weaker than with the triangular obstacles. The effect of the quadrangular obstacles on flame velocity is mainly influenced by gas flow at the flame front. In triangular obstacles, the shear layer became prominent in the later stage of the explosion process and this contributes to enhancing the flame velocity and overpressure.

- **Keywords:** Gas explosion analysis; Hydrogen fuel; Process safety; Hydrogen safety; Methane explosion

Zhuang Liu, Dachao Ma, Liwu Liang, Xuan Hu, Mengxue Ling, Zhou Zhou, Lizhong Fu, Zheng Liu, Qingge Feng. *Co-hydrothermal dechlorination of PVC plastic and bagasse: Hydrochar combustion characteristics and gas emission behavior*. Pages 88-99.

Hydrothermal treatment (HTT) of polyvinyl chloride (PVC) can efficiently remove chlorine (Cl) to produce low Cl hydrochar for solid fuel. This work performed co-hydrothermal treatment of PVC recycled plastics (PVCR) with biomass, then tried to reveal the combustion behavior and Cl migration behavior during combustion of PVC-derived hydrochar. It is shown that the hydrothermal temperature was the dominant factor affecting the degradation and dechlorination of PVCR. Treated at 220 ℃ for 60 min, the dechlorination efficiency of PVCR was 4.88 wt% and it was significantly increased to 34.09 wt%, 28.60 wt% and 32.50 wt% when PVCR was co-treated with bagasse, bagasse + high impact polystyrene (HIPS) and bagasse + acrylonitrile butadiene styrene (ABS), respectively. The substitution of Cl by hydroxyl (-OH) and elimination were two main dechlorination pathways. Bagasse could provide abundant -OH so as to promote the dechlorination of PVCR. Interestingly, in the combustion of PVCR and hydrochars, the Cl was mainly released in the form of HCl at lower temperature combustion stage but C-Cl mostly emitted at higher temperature combustion stage. The emitted Cl species strongly depends on the Cl content in hydrochar and combustion temperature, but did not show relevance to the existence form of Cl in hydrochar. Hydrothermal dechlorination could sharply reduce HCl emission.

- **Keywords:** PVCR; Bagasse; Co-hydrothermal dechlorination; Hydrochar combustion; Cl migration

Senpei Wang, Zhan Li, Qin Fang, Haichun Yan, Yang Liu. *Numerical simulation of overpressure loads generated by gas explosions in utility tunnels*. Pages 100-117.

Studies of overpressure loads are essential to mitigate the potential hazards of public safety induced by gas explosion accidents. Based on the computational fluid dynamics (CFD) code FLACS, numerical models of gas explosions in large-scale tunnels were developed and verified by comparing with testing data. Numerical simulations of gas explosions in confined and side-vented utility tunnels were carried out. The effects of the venting condition, gas cloud volume, and ignition position were analyzed and discussed. It is found that gas explosions in utility tunnels can be divided into three stages according to the pressure and flame development, i.e., the combustion-induced rise stage, oscillation rise stage, and oscillation decline stage. The pressure oscillation is significant, and a side vent near the tunnel end can reduce the peak pressure by 42~78% and the oscillation peak by 35~87%. The peak pressure, oscillation peak, and duration of oscillation rise stage varied significantly with the gas cloud volume. When the premixed gas cloud is ignited at the 1/4 L, the peak pressure and oscillation peak reach the maximum of 1242.5 kPa and 490.4 kPa for confined cases, which are one time higher than those of side-vented cases. What is more, based on the equivalent single degree of freedom (SDOF) approach in the elastic range, the dynamic effects of gas explosions in utility tunnels are figured out, and suggestions for engineering practice are proposed.

- **Keywords:** Gas explosion; Utility tunnel; Numerical simulation; Overpressure loads; Flame development

Zixiang He, Yusheng Cheng, Xiaobin Liao, Jing Yu, Xina Lin, Huan Qi. *Which pre-oxidation methods to choose? From perspective of DBPs formation and toxicities reduction*. Pages 118-125.

Pre-oxidation have been widely applied in drinking water treatment plants with micro-polluted water as water sources. In this study, the effects of three commonly used oxidants (ozone, chlorine, and potassium permanganate) on disinfection by-products (DBPs) formation from micro-polluted water during subsequent chlorination and chloramination were investigated. Moreover, the toxicities of treated water were also compared. In addition, principal component analysis was applied to clarify the main components that contributed to DBPs generation. The results demonstrated that all the selected oxidants could reduce DBPs to some extent, but the species and amounts were quite different. Pre-KMnO4 greatly reduced haloacetic acid (HAAs) formation in subsequent chloramination; the removal rate reached up to 45.2%. Pre-HClO could produce trihalomethane (THMs) and HAAs directly, and its effect on DBPs reduction during subsequent disinfection processes was limited. Pre-O3 performed best on N, N-dimethyl nitrosamine (NDMA) reduction during subsequent chloramination; the corresponding removal rates were 49.7%. In addition, pre-O3 significantly reduced UV254 and SUVA. Pre-KMnO4 transferred more organic matter to cationic components (24%), while the highest polar component augmentation was observed during pre-HClO (15%). Based on the analysis of total toxicity of formed DBPs, pre-O3 performed best on toxicity reduction no matter subsequent chlorination or chloramination, which decreased by 25.8% and 46.4%, respectively. The principal component analysis showed that DBPs has a weak correlation with regular water quality parameters, but related with specific organic fractions. The results of this paper had significant guidance for the selection of pre-oxidation methods in drinking water treatment plants for this kind of water sources.

- **Keywords:** Disinfection by-products; Pre-oxidation; Toxicity; Chlorination; Chloramination

Dongxu Ouyang, Jingwen Weng, Mingyi Chen, Yu Zhu, Jian Wang, Zhirong Wang. A comparative study on safety and electrochemical characteristics of cylindrical lithium-ion cells with various formats. Pages 126-135.

The present work carries out a comparative study to illustrate the safety performance of two new-format cells (22650 and 26650) in the thermal runaway tests induced by over-heating and overcharge tests, referred by the traditional 18650 cells. In addition, a long-term cycling test is also performed to evaluate the electrochemical characteristics of the three cells. When charged to the same capacity (1700 mAh), the cell with a larger size demonstrates comparative gentler thermal runaway behaviors during the over-heating, with a longer time to thermal runway and a higher temperature to thermal runaway. The thermal runaway of the fully charged 26650 cell lags behind that of 18650 and 22650 cells in the over-heating tests; that is, the 26650 cell shows the best thermal safety performance among the three kinds of cells. The safety performance of the 26650 cell is also more competitive than 18650 and 22650 cells during overcharging, with a larger SOCend illustrated when the interior safety devices take effects. At last, the 26650 cell shows more promising electrochemical features, demonstrating a larger absolute capacity and a slighter degradation over the long-term cycling, in comparison with 18650 and 22650 cells.

- **Keywords:** Lithium-ion cell; Thermal runaway; Overcharge; Cycling

Yan Cao, Hayder A. Dhahad, Hossein Esmaeili, Mohammadreza Razavi. *MgO@CNT@K2CO3 as a superior catalyst for biodiesel production from waste edible oil using two-step transesterification process*. Pages 136-146.

Due to limited fossil fuel resources and greenhouse gas emissions, the use of biodiesel is increasing. In this study, biodiesel was produced from waste edible oil (WEO), as a low-cost oil, using MgO and MgO@CNT@K2CO3 catalysts. The MgO@CNT@K2CO3 catalyst was first synthesized in this study and used to produce biodiesel. To this end, the features of these catalysts were studied using FTIR, BET, XRD, EDX, SEM, and Map analyses. The results indicated that both catalysts have high catalytic activity with mesoporous structures. Due to the high content of free fatty acid (2.43 wt%) in WEO, a two-step transesterification process was used to convert WEO to biodiesel. In the first step, hydrochloric acid homogeneous catalyst was employed to reduce the FFA content and then in the second step, MgO and MgO@CNT@K2CO3 heterogeneous catalysts were used to generate biodiesel. The highest biodiesel yields using MgO and MgO@CNT@K2CO3 were 94.26% and 98.25%, respectively, which were achieved at a catalyst concentration of 4%, temperature of 65 °C, and methanol/oil ratio of 24:1 and 20:1 after 5 and 4 h for MgO and MgO@CNT@K2CO3, respectively. The MgO@CNT@K2CO3 showed the highest biodiesel yield ever achieved from WEO. Also, the physical features of biodiesel were investigated and the results demonstrated that the biodiesel produced are in accordance with ASTM D6751 and EN14214 standards. Moreover, kinetic and thermodynamic studies showed that the transesterification reaction is endothermic and non-spontaneous. Therefore, MgO@CNT@K2CO3 is proposed as a strong and cost-effective catalyst for biodiesel generation from WEO on an industrial scale.

- **Keywords:** Biodiesel; MgO; MgO@CNT@K2CO3; Two-step transesterification process; Waste edible oil

Jana Růžičková, Helena Raclavská, Dagmar Juchelková, Marek Kucbel, Karolina Slamová. *The origin of potential precursors of secondary organic aerosols during combustion of biochar and softwood in residential heating*. Pages 147-161.

Compounds that are potential precursors of secondary organic –aerosols account for up to 33.4 ± 7.1 mg/m3 in softwood combustion emissions, while biochar can be considered zero-emission fuel (0.18 ± 0.06 mg/m3). The characteristic feature of gaseous emissions from biochar combustion is the presence of n-alkanes (70.3 ± 6.6 μg/m3), which arise from the thermal degradation of waxes, cuticles, and plant lipids. In addition to alkanes, carboxylic acids (4.9 ± 0.2 μg/m3) are present in biochar emissions at significantly lower concentrations. In deposits from biochar combustion (6.1 ± 0.8 g/kg), the internal parts of the boiler capture 20% more organic compounds than in wood-burning deposits (4.84 ± 0.91 g/kg). The greater uptake of organic compounds in biochar combustion deposits (513.8 ± 6.2 g/kg) than in softwood (382.7 ± 27.3 g/kg) is related to the higher elemental carbon content in biochar. The organic compounds present in deposits from biochar are mainly methyl ketone, fatty acids such and alkanes. In deposits from softwood, the compounds of chemical groups of phenols, anhydrosaccharides and acetic acids are present. The novelty lies in identifying and determining the quantity of organic compounds that form precursors of the solid organic aerosols in the combustion of biochar.

- **Keywords:** Secondary organic aerosols; Residential heating; Biochar; Emissions; Organic carbon

Feng Wu, Hao Yu, Xuhai Pan, Xiaowei Zang, Min Hua, He Wang, Juncheng Jiang. *Experimental study of methanol atomization and spray explosion characteristic under negative pressure*. Pages 162-174.

Leakage of methanol under negative pressure may cause high dangerous spray explosion in the process industry. The explosion characteristics of methanol spray under the combined effects of multi-factor have not yet been studied. Hence, combined effects of spray concentration (198.0–514.8 g/m3), ambient temperature (298.15–323.15 K) and injection pressure (13–21 bar) on atomization and spray explosion of methanol (308.15 K) in 20 L spherical vessel under negative pressure (0.80–1.00 bar) were studied in this paper. The results showed that the decrease of methanol concentration, the increase of ambient temperature and injection pressure all promoted the breakage of methanol spray with linear trend. Based on the negative pressure, the effect weights of concentration, ambient temperature, and injection pressure were 113.7 μm/bara, 243.3 μm/bara, 64.24 μm/bara, respectively. The "peak plateau" of explosion temperature lasted for 237.6 ms due to the multi-point source ignition. In contrast to the explosion pressure change, the temperature of methanol spray slightly decreased in delayed ignition region. The increase of spray concentration provided more combustibles and contributed to the spray explosion when the methanol concentration was below 356.4 g/m3. As the concentration continued to rise, the maximum explosion pressure under room pressure (0.1 bar) decreased inhibited by the poor oxygen, while the maximum explosion pressure under negative pressure (0.80–0.95 bar) slowly increased. The increase of ambient temperature promoted the maximum explosion pressure, temperature and the rate of pressure rise, especially the promotion under negative pressure, was more significant. The variation of the maximum explosion pressure and maximum rate of pressure rise was consistent with that of the spray particle size when influenced by injection pressure. The experimental results showed that the methanol spray was more explosive and dangerous under negative pressure.

- **Keywords:** Negative pressure; Methanol spray; Particle size; Explosion characteristics; Closed vessel

Yang Liu, Lixing Zhou. *Hydrodynamic modeling of non-swirling and swirling gas-particle two-phase turbulent flow using large eddy simulation*. Pages 175-187.

Flow structures of non-swirling and swirling particle-laden turbulence are modeled using the large eddy simulation. Four-way coupling to reveal the interaction mechanism of gas to particle, particle to gas and particle-particle collisions is adopted by a new proposed subgrid scale (SGS) particle kinetic energy-granular temperature model. Evolution of particle vortices, particle coherent structures and particle dynamics are predicted numerically, and comparisons are also conducted. Predictions are in good agreement with experimental measurements. For non-swirling flows, the typical coherent structures, and larger vortices at downward region of gas flow are dominantly. However, particle transport characteristics are significantly different, distinctly coherent structures and more vortices have not been generated in additions to fewer ones at far distance from entrance. Meanwhile, fewer coherent structures and vortices that dispersed at corner recirculation are observed for swirling flow. Compared to gas flow, the number of particle vortices is less and Reynolds stress and kinetic energy transport behaviors of particle flow are relatively independent due to inertia. Gas fluctuations of shear stresses are approximately twice greater than those of particle in non-swirling flows. A novelty finding is that turbulent fluctuations and instantaneous gas vortices of non-swirling flow are stronger than swirling case.

- **Keywords:** Large eddy simulation; Particle subgrid scale model; Interaction mechanism; Swirling; Two-phase turbulent flow

S. Pavithra, T. Veeramani, S. Sree Subha, P.J. Sathish Kumar, S. Shanmugan, Ammar H. Elsheikh, F.A. Essa. *Revealing prediction of perched cum off-centered wick solar still performance using network based on optimizer algorithm*. Pages 188-200.

A sincere effort has been made to engineer a perched cum off-centered wick solar still (PCWSS) in the present work. The daily average efficiency with hourly prediction distillate yield of the PCWSS has used those artificial neural networks (ANNs) tool with Harris Hawk's Optimizes (HHOs) technique. HHO performance with ANN simulated as an optimal parameter to grab preyed. An experimental performance predicting the system's productivity is associated by dual supplementary mockups as vectors gadget, tradition ANN. HHO-ANN approach results are compared with the experimental observations (one year) of the solar still. Radial Basis Function (RBF) and Feed Forward (FF) have been used ANN structures to estimate hourly distillate yield and efficiency of the system is 59.78%. Evaluating the R2, RMSE, MRE, MAE, EC, OI, CRM analysis of prediction models was based on numerical error conditions. Optimized the analysis of PCWSS with a model as HHO-ANN used optimal parameter values has prediction accuracy associated with ANN and the competence for HHO. Annual analysis based on the HHO - ANN structures predicted the hourly distillate yield with mean error varying from 8.13% and 6.1%. The error for the monthly average prediction of distillate yield is from 0.95% to 1.12%, respectively. HHO – ANN has been used with the best accuracy in predicting the PCWSS invention associated with tangible experimental outcomes.

- **Keywords:** Machine learning; ANN models; Distillate yield; Efficiency; Radial basis function; Forward feedback

Liangqiong Peng, Wenjun Long, Wenhua Zhang, Bi Shi. *Leaching toxicity and ecotoxicity of tanned leather waste during production phase*. Pages 201-209.

This paper investigated the environmental impact of leather from production phase via identifying the hazardous substances (such as HCHO, Cr[VI]), leaching toxicity and ecotoxicity, with special emphasis on chrome or chrome-free. The hazardous substances of concern in various tanned leather waste from processing and commercial product were found lower than the present criterion for the eco-label product, different from the leaching toxicity and ecotoxicity. Several of the chrome-leather samples might be classified as hazardous waste for total chrome leached beyond the limitation though no Cr(VI) was leached out. Whereas the ecotoxicity toward photobacterium phosphoreum of leather samples from technology flow indicated chrome-tanned samples (S1–S3) was more toxic than corresponding chrome-free samples (S4–S6), confirming the crucial environmental impact of the tanning procedure. The increased toxicity of finished leather (S3 and S6) also revealed the significance of the finishing procedure in developing environment-friendly leather products. The multiple linear regression further demonstrated the positive correlations of the ecotoxicity of leather with leached total Cr, HCHO, and anionic polyelectrolyte. These results discerned the crucial procedures and chemicals to improve the process safety of leather.

- **Keywords:** Tanned leather waste; Leather-making technology; Hazardous substances; Leaching toxicity; Ecotoxicity assessment

Ayse Yuksekdag, Borte Kose-Mutlu, Mark R. Wiesner, Ismail Koyuncu. *Effect of pre-concentration on membrane solvent extraction process for the recovery of rare earth elements from dilute acidic leachate*. Pages 210-220.

Pre-concentration and separation processes of Rare Earth Elements (REEs) were investigated in terms of several factors. Nitric acid leachate of e-waste was first pre-treated by increasing pH and filtering through microfiltration. For pre-concentration, pre-treated leachate was concentrated by nanofiltration. While a 70% permeate recovery ratio was kept constant, the rare earth elements concentrations were triplicated under optimum conditions. A flat sheet supported liquid membrane process with a polyvinylidene fluoride (PVDF) support membrane was successfully used to extract REEs from the pre-treated leachate. Of the two extractants evaluated, bis-2-ethylhexyl phosphoric acid (D2EHPA) displayed a higher REE separation efficiency than did di-2,4,4,-trimethylpentyl phosphinic acid (Cyanex 272). However, Cyanex 272 separated Sc more selectively. For direct membrane solvent extraction (MSX) and MSX with pre-concentration, pre-treatment pH and D2EHPA concentrations were optimized at values of 1.5% and 15%, respectively. When comparing the results of MSX for direct and pre-concentrated configurations, it was seen that REEs and HREEs recoveries were increased 10% and 30% in MSX with pre-concentration at the end of single-stage MSX. Pre-concentration not only increased the MSX process efficiency but also enabled acid recovery from nanofiltration permeate. A more environmentally friendly and economical process scheme was proposed, including acid recovery from both NF filtrate and post-MSX leaching residue by two different membrane distillation configurations.

- **Keywords:** Mixed e-waste; Rare earth elements; Nanofiltration; Supported liquid membrane; Separation

Samer Fawzy, Ahmed I. Osman, Charlie Farrell, Ala'a H. Al-Muhtaseb, John Harrison, David W. Rooney. *Kinetic modelling for pyrolytic degradation of olive tree pruning residues with predictions under various heating configurations*. Pages 221-230.

Herein, the aim was to develop an in-depth understanding of the kinetic behaviour of olive tree pruning residue (OTPR), an abundant agricultural waste, during pyrolysis. Thermal analysis at 1, 2, 4, 6 and 10 °C.min−1 was performed using TGA-thermogravimetric analysis, with the results subsequently used to determine the OTPR's kinetic thermal breakdown behaviour. Furthermore, advanced kinetics and technology solutions (AKTS) thermo-kinetic tool was applied to investigate the kinetic behaviour of OTPR and to generate kinetic predictions for various heating configurations. Friedman's method was the main approach used to evaluate the kinetic parameters. For comparison, other established kinetic modelling techniques, such as ASTM-E698 and Flynn-Wall-Ozawa (FWO) methods, were applied. The ASTM-E698 approach yielded an apparent activation energy (Ea) of 172.09 kJ.mol−1, whereas the FWO method yielded an Ea range from 38 to 172 kJ.mol−1. Finally, the differential iso-conversional approach yielded Ea values ranging between 85 and 191 kJ.mol−1. Kinetic predictions were then developed for isothermal, non-isothermal, and stepwise configurations using the kinetic parameters obtained via Friedman's model. The forecasts shed light on optimising production throughput in a variety of reactor configurations.

- **Keywords:** Agricultural residues; Kinetic modelling; Thermal predictions; Climate change mitigation; Biochar

Matteo Iaiani, Riccardo Sorichetti, Alessandro Tugnoli, Valerio Cozzani. *Projectile perforation models for the vulnerability assessment of atmospheric storage tanks*. Pages 231-246.

Chemical and process plants storing large quantities of hazardous materials (flammable and/or toxic) may be attractive targets of intentional malicious attacks threatening the life and health of workers and population, as well as the environment and the availability of critical infrastructures. Quantification of the vulnerability of industrial facilities against shooting attacks received scarce attention in the context of Security Vulnerability Assessment (SVA) or Security Risk Assessment (SRA) methodologies. Specific damage models for projectile impact on equipment items storing relevant quantities of hazardous materials are not available in the literature. The current study aims at filling this gap by reviewing a wide set of empirical and analytical perforation models and validating them against experimental data from ballistic experimental tests. According to specific statistical parameters, the most suitable perforation models were selected in order to be used in the definition of quantitative methods for the analysis of the shooting attacks to atmospheric storage equipment. The application of the selected models to the assessment of the vulnerability to perforation of steel atmospheric storage tanks showed important differences between handguns and rifles as regards the thickness that can be successfully perforated. The results allowed for the definition of inherent safety thresholds for the perforation thickness that can be used in the context of vulnerability assessment of critical assets within SVA/SRA.

- **Keywords:** Security; Chemical and process industry; Shooting; Projectile impact; Perforation model; Ballistic limit velocity

Yuan Mei, Jian Shuai. *Research on natural gas leakage and diffusion characteristics in enclosed building layout*. Pages 247-262.

There are many people in urban construction areas, and natural gas leakage can potentially cause serious accident consequences. Predicting the consequences of gas dispersion is important to react rapidly and adequately in the event of an incident. Currently, computational fluid dynamics (CFD) models are an important tool to predict gas dispersion. However, in most cases, considering computational cost, the building layouts is ignored, so the flow field influence near the building area cannot be considered. In this research process, a realizable k-ε turbulence model is used to simulate the natural gas leakage process in a typical building layout (enclosed building layout), while focusing on wind speed and the leakage position. The validity of realizable k-ε turbulence model is verified by experimental data. The results show that under conditions of high wind speed (wind speed≥ 6 m/s), the reverse vortex formed by the shear flow of wind can cause the natural gas cloud to sink. When the leak hole is located in the influence area of the turbulent vortex, it easily induces R-H instability. When combined with the stronger K-H instability at high wind speeds, natural gas clouds may accumulate. This then leads to serious leakage accidents, knowledge of which may be the key component of emergency management during an accidental natural gas leakage. The research results can guide the building layout plan and gas pipeline construction to prevent accidents.

- **Keywords:** Buildings; Natural gas; Leakage diffusion; Flow field characteristics; Gas cloud accumulation

Sálvio Lima de Carvalho Neto, Juliano Cesar Toledo Viviani, Silvio Edegar Weschenfelder, Maria de Fatima Rodrigues da Cunha, Aloisio Euclides Orlando Junior, Byron Rosemberg dos Santos Costa, Luciana Prazeres Mazur, Belisa Alcantara Marinho, Adriano da Silva, Antônio Augusto Ulson de Souza, Selene Maria Arruda Guelli Ulson de Souza. *Evaluation of petroleum as extractor fluid in liquid-liquid extraction to reduce the oil and grease content of oilfield produced water*. Pages 263-272.

This work aims to evaluate the use of petroleum as a solvent in the liquid-liquid extraction of oil and grease content from oilfied produced water. Initially, tests were performed with synthetic effluent, using cyclohexanecarboxylic acid as model compound through the study of physical-chemical parameters: pH, temperature, stirring speed and time, petroleum type and concentration, and initial concentration of naphthenic acids. Afterwards, the process was evaluated for the removal of oil and grease content from a real oilfield produced water sample. The pH and petroleum concentration proved to be significantly influential in removing cyclohexanecarboxylic acid from the synthetic produced water (ANOVA). The greater the amount of petroleum present, the greater the efficiency. By acidifying the synthetic effluent, the efficiency of removing these naphthenic acids from the synthetic produced water was increased. Response surface methodology (RSM) evaluated these two factors. On the other hand, the initial concentration of cyclohexanecarboxylic acid and petroleum type did not presented great influence on the obtained results, indicating robustness of the process. The methodology carried out with synthetic effluent proved to be efficient in removing the oil and grease content from real effluent (≈ 60% of removal at pH range 2–5).

- **Keywords:** Naphthenic acids; Synthetic effluent; Real effluent; Oil and grease; Produced water treatment

Aobo Liu, Michael A. Delichatsios, Yiannis A. Levendis. *On the trajectory and reach of fire-suppressant liquid nitrogen droplets released from a spray nozzle*. Pages 273-284.

Liquid nitrogen (LN2) can be used to supplement or replace currently used fire extinguishers in challenging fire situations. This environmentally-benign cryogenic fluid can be produced readily from deep refrigeration of air. This manuscript addresses the application of liquid nitrogen to fires through a nozzle. Its aim is to investigate the survivability of LN2 droplets, following breakup of the jet exiting the nozzle, and the amount of liquid that reaches a target. Numerical simulations were carried out to explore the effects of relevant parameters, such as the initial droplet size and velocity, the droplet injection angle, and the thermal radiation on the droplet flight distance and the liquid droplet mass. The results indicate that all these parameters influence the fate of the LN2 droplets. Coarse atomization, high initial velocities, short nozzle-to-target distances, and shallow jet angles maximize the amount of the cryogen delivered to the target. A small-scale experiment was performed to test the results of the calculations. The comparison of the experimental results and the theoretical calculations was deemed satisfactory. In both cases the reach of the liquid droplets was in the order of 1 m from the nozzle, for an initial droplet velocity in the neighborhood of 20 m/s as measured in the experiments.

- **Keywords:** Liquid nitrogen; Droplets; Spray nozzle; Fire suppression

Jialong Zhu, Ruina Li, Zhong Wang, Shuai Liu, Hui Lv. *Decoupled analysis of the effect of hydroxyl functional groups on delay of ignition with fictitious hydroxyl*. Pages 285-294.

The delay of ignition (DOI) affects engine performances and the fundamental reasons that affect DOI have not been fully explained. In this paper, taking biodiesel mixed with methanol as an example, the effect of the hydroxyl (-OH) functional group in the fuel on the DOI was studied. Through thermogravimetric analyzer and constant volume combustion chamber (CVCC), the activation energy and DOI of different blending ratios (0%, 10%, 20% and 30%) of biodiesel/methanol mixed fuel were determined. Using the fictitious hydroxyl (FOH-) method, the low-temperature oxidation of biodiesel/methanol/FOH- and the reaction path of ignition in the cylinder were analyzed. The results show that when the methanol blending ratio is less than 30%, as the blending concentration of FOH- groups increases, the low-temperature oxidation reaction activity of the mixed fuel increases, and the activation energy decreases. The physical and chemical effects of -OH can prolong and shorten DOI, respectively, and the influence of physical effects is more important than chemical effects. For every 10% increase in -OH functional group concentration, the DOI of biodiesel/methanol mixed fuel increases by 1.4%.

- **Keywords:** Activation energy; Delay of ignition; Hydroxyl group; Chemical reaction path

Navid Nedaei, Saeid Azizi, Leili Garousi Farshi. *Performance assessment and multi-objective optimization of a multi-generation system based on solar tower power: A case study in Dubai, UAE*. Pages 295-315.

This paper designs and evaluates an innovative multigeneration system based on a heliostat solar field that is a combination of closed Brayton cycle, absorption refrigeration cycle, humidification and dehumidification desalination, and proton exchange membrane electrolyzer. Thermodynamic and exergoeconomic analyses are performed for the performance assessment. Moreover, the grey wolf optimization algorithm in different multi-objective optimization scenarios is implemented to obtain the optimum operating conditions and desirable performances. According to the obtained results, the simulation at the base operating conditions is led to generating 8.32 MW of power, 3.16 kg/s of freshwater, 8.37 MW of cooling load, and 0.22 kg/h of hydrogen with 39.15% exergy efficiency and 8.81 $/GJ sum unit cost of products. Moreover, the lowest payback period and maximum profitability are related to the electricity price of 0.07 $/kWh, with a payback period of 2.93 years. Also, at the optimum point, the exergetic efficiency with SUCP and freshwater production rate are considered obtained to be 45.09%, 8.27 $/GJ, and 3.89 kg/s. Finally, the proposed system performance was evaluated for a case study of Dubai, UAE. It is resulted that the maximum net power obtained in May during a yearly operation by about 7.40 MW with exergetic efficiency of 38.70%.

- **Keywords:** Case study; Desalination; Multigeneration system; Multi-aspect analysis; Solar energy

Xin Zhang, Yong Pan, Yuqing Ni, Xianghui Shi, Juncheng Jiang. *Atomistic insights into the pyrolysis of methyl ethyl ketone peroxide via ReaxFF molecular dynamics simulation*. Pages 316-324.

Methyl ethyl ketone peroxide (MEKP) has caused the largest number of incidents among organic peroxides due to the thermal risk. However, the mechanisms of pyrolysis reactions are still unclear. Herein, the pyrolysis of the MEKP dimer and monomer, the predominant existence forms of commercial MEKP, is investigated via the ReaxFF molecular dynamics simulations. The results show that there exist two-stage reactions,

consistent with the reported experiments. In the primary reaction, large numbers of butanone, O2, and water are generated. The consumption of O2 will trigger the secondary exothermic reaction, leading to the generation of many small molecules such as H2O, CH2CH2, CH2CO, CO2, and CO. The products of the MEKP dimer and monomer are the same. To clarify the detailed mechanisms of pyrolysis, we investigate the pathways of initial reactions, most of which are associated with the OO bond scission. The initial reactions are composed of the splitting decomposition and self-reactions with the MEKP itself or the radicals. In addition, the main generation and consumption pathways of the major species are tracked, including butanone, O2, and water. Finally, the apparent activation energies calculated by ReaxFF simulations are consistent with the experimental results. These findings are expected to provide fundamental guidance for the process safety in the production, transportation, and storage of organic peroxides.

- **Keywords:** Methyl ethyl ketone peroxide (MEKP); Pyrolysis; Reactive molecular dynamics; Reaction pathway; Organic peroxide

Jialu Fan, Xianbo Sun, Yongdi Liu, Dongye Zhao, Xiaodi Hao, Wen Liu, Zhengqing Cai. *New insight into environmental photochemistry of PAHs induced by dissolved organic matters: A model of naphthalene in seawater.* Pages 325-333.

The photochemical behavior of a model PAH, naphthalene, was investigated under simulated sunlight irradiation with different dissolved organic matter (DOM) in seawater. The results revealed that naphthalene was prone to direct photolysis (Φd = 1.34 × 10-3) and could be degraded by 3DOM*/1O2-induced reactions with fulvic acid (FA) and humic acid (HA) at low concentrations. However, the DOM at a high level dramatically decreased the kobs due to the higher light attenuation and radical competition effect. The presence of FA resulted in lower 3DOM*/1O2 generation and quantum yield compared with HA, but it achieved higher degradation kinetics due to the higher reactivity between 3FA* and naphthalene and their lower binding effect. The naphthalene degradation in natural water with different depths and DOM were modeled based on the experimental results, which revealed the important role of indirect photolysis initiated by inorganic constituents. Moreover, several degradation intermediates were identified by GC-MS and three possible pathways were proposed. The Quantitative Structure Activity Relationships (QSAR) evaluation revealed that some intermediates are more toxic than original naphthalene. This study offers further insights into the photochemical behavior of PAHs, which will facilitate our understanding of the persistence and ecological risks of organic contaminants in natural waters.

- **Keywords:** Polycyclic aromatic hydrocarbons; Photochemical degradation; Reactive species; Modeling

Matteo Iaiani, Alessandro Tugnoli, Valerio Cozzani. *Identification of reference scenarios for security attacks to the process industry*. Pages 334-356.

The possibility of inducing severe security-related events with damage to people, property, and the environment by deliberate malicious attacks to chemical and process plants handling large quantities of hazardous materials received an increasing attention in recent years. The identification of the credible security scenarios is required by Security Vulnerability/Risk Assessment (SVA/SRA) methodologies. However, the current availability of supporting tools is limited. This may hinder a proper management of the risks, especially in the European context where security threats are only marginally recognized under the Seveso legislation. The present study aims at supporting a harmonized identification of the scenarios triggered by deliberate malicious physical attacks to chemical and process plants. An approach based on Bow-Tie formalism is

proposed to identify reference security scenarios. The Bow-Tie diagram is used to link the attack modes (Attack Tree) to the relevant release scenarios (Security Events) and to the physical damage scenarios (Event Tree). Reference Bow-Tie diagrams were defined considering substances commonly present in process plants (e.g. flammable substances and oxidizing solids). The validation of the reference scenarios (both attack scenarios and physical damage scenarios) was provided by the analysis of more than 20 security-related incidents that occurred in chemical and process facilities worldwide in the last 50 years. Application to a case-study proved the effectiveness of the results achieved in supporting SVA/SRA studies and in promoting integration among safety and security management.

- **Keywords:** Major accident hazards; Hazardous substances; Security; Bow-tie diagram; Scenario identification

Ali Nawaz, Ikram ul Haq, Kinza Qaisar, Burcu Gunes, Saleha Ibadat Raja, Khola Mohyuddin, Haseeb Amin. *Microbial fuel cells: Insight into simultaneous wastewater treatment and bioelectricity generation*. Pages 357-373.

Burgeoning industrialization has escalated the energy demand and amplified the insistence on depleting petroleum-based reservoirs. Subsequently, this has imposed a study to pinpoint renewable alternative sources. Employing renewable resources promotes energy production coupled with environmental sustainability. Microbial fuel cells (MFCs) have an encouraging role in producing sustainable and viable electrical energy. It transforms chemical energy into electrical energy with the assistance of microorganisms acting as biocatalysts. It is an emerging technology that has the potential to treat wastewater with bioelectricity production simultaneously. However, scaling up this technology is a major challenge as a plethora of technical constraints limits its application in the real world. This review highlights MFC performance in terms of power generation by utilizing various wastewaters as substrate. Moreover, it sheds light on different MFC designs, mechanisms, and parameters affecting MFC performance along with their pros and cons to generate maximum power output. It concludes possible ways to combat its drawbacks and discusses its future prospects.

- **Keywords:** Microbial fuel cell, wastewater treatment; Bioelectricity; Biocatalysts; Electrogens; Reactor design

Yang Ni, Chun-chen Nie, Shun-xiang Shi, Xiang-nan Zhu. *Effect of mechanical force on dissociation characteristics of cathode materials in spent lithium-ion batteries*. Pages 374-383.

With the rapid growth of the demand for lithium-ion batteries (LIBs), the treatment challenges of spent LIBs continue to increase. The dissociation characteristics of the electrode materials by impact crushing and shear crushing were studied. The liberation characteristics of each size particles and over crushing rule of aluminum (Al) foil were analyzed. The results show that both shear crushing and impact crushing can achieve effective liberation of electrode materials. The rapid liberation of cathode material can be achieved by shear crushing in 5 s, the particle size of the shear crushed products is mainly concentrated in + 2 mm and − 0.074 mm, and the degree of liberation increases to 69.29% at 40 s. Meanwhile, the liberation caused by impact crushing mainly occurs within 5–20 s, the liberation degree increases sharply from 1.36% to 49.51%, and final liberation degree can reach 62.68% with 40 s crushing. In addition, the over crushing of Al foil is inevitable in impact crushing and shear crushing, and the Al content of − 0.074 mm crushing products of shear crushing and impact crushing fluctuates within 2.4%− 3.5%. This study provides a feasible technical approach for the safe and environmentally friendly dissociation of electrode materials in spent LIBs.

- **Keywords:** Spent lithium-ion batteries; Cathode material; Crushing; Dissociation characteristics

Jintao Gao, Xintuo Qu, Xi Lan, Yu Li, Zhancheng Guo. *A green method for solidification and recovery of soluble sodium in red mud via super-gravity*. Pages 384-391.

Red mud produced in the Bayer process is an ultrafine solid waste containing various metallic elements, which is hazardous to the environment because of its high alkalinity caused by the soluble sodium (Na). In this study, a green method for efficiently solidification and recovery of soluble sodium to eliminate high alkalinity of red mud via super-gravity was developed. Iron-slag melting separation from red mud was firstly conducted at 1523 K, where the Fe was fully recovered into metallic iron and almost all the Na was enriched into the Na-rich slag. Subsequently, the Na was selectively solidified into a stable phase of anorthite at 1373–1323 K, all of which were efficiently separated from the Na-rich slag at 1323 K via super-gravity, where the recovery ratio of Na in anorthite was up to 97.09%. Compared to the red mud, the leaching rates of Na+ in the anorthite and residue were significantly decreased to 0.01% and 0.05%, and the pH of both products was decreased to 8.1–8.4. It was confirmed that the high soluble sodium in red mud was efficiently solidified and recovered into a stable phase of anorthite, and the high alkalinity was fully eliminated in both products which are environmentally friendly.

- **Keywords:** Red mud; Soluble sodium; Solidification; Green recovery; Anorthite

Dora Lawrencia, Lay Hong Chuah, Phatchani Srikhumsuk, Phaik Eong Poh. *Biodegradation factors and kinetic studies of point-of-use water treatment membrane in soil*. Pages 392-408.

Point-of-use (POU) water treatment technology in developing countries and rural regions is more feasible than a centralized water treatment system due to the high cost of pipe distribution. The water filtration system can provide quick and easy access to water with low maintenance and higher pathogen removal among POU technologies. However, non-biodegradable polymeric materials for water filtration membranes raise environmental concerns due to their problematic disposal. There is increasing research on biodegradable membrane material, but the validation of biodegradability is still lacking as measuring weight loss does not guarantee the complete mineralization of biodegradable membrane. This review aims to discuss various abiotic and biotic factors affecting polymer degradability in soil or compost, gather and evaluate existing studies on biodegradable filtration membrane and identify existing methods used to validate membrane biodegradability. Different kinetic models used to understand the biodegradation mechanism at different stages were studied. Factors affecting morphology and surface properties affect biodegradability. Membrane biodegradation follows a first-order model followed by a lag phase. Finally, future studies of biodegradable filtration membrane could include CO2 quantification and phytotoxicity studies, exploring different additives and membrane formulations to balance membrane performance and degradation ability, and lastly, conducting LCA and TEA to assess overall sustainability.

- **Keywords:** Water scarcity; Membrane filtration; Biodegradability; Soil; Compost; Kinetics; Waste management

Daniel Eastvedt, Greg Naterer, Xili Duan. *Detection of faults in subsea pipelines by flow monitoring with regression supervised machine learning*. Pages 409-420.

This study investigates the relationship between pressure change, velocity change, and temperature of crude oil through a pipeline and presents a method of using a regression supervised machine learning (ML) algorithm to detect faults. A representative dataset of crude oil flow is generated by computational fluid dynamics (CFD) and used to train the algorithm to develop a model of fluid behavior under normal pipeline operations over a range of typical flow rates and temperatures. CFD data are then collected under several simulated fault conditions: leaks of 10% and 20%, and a 50% restriction to flow, by nominal pipe cross-sectional area. This study demonstrates that the ML algorithm can be trained to model the system under normal conditions, thereby successfully recognizing a fault condition as non-conforming and indicative of a statistically significant change in pipeline operation. It is further able to identify the fault type based on the pattern observed in the new data. It is shown that ML may be a safe, low-cost, and accurate method of monitoring a subsea pipeline for optimal performance and fault detection without the need to introduce special equipment to a subsea pipeline network, providing an avenue for enhanced process safety and protection of ocean environments. This paper demonstrates that the application of ML to the monitoring of pipeline networks could provide valuable contributions to the industry in terms of safety, cost, and environmental protection.

- **Keywords:** Machine learning; Pipeline monitoring; Fault detection; Leak and flow restriction risk; Process safety

Yang Wang, Jingde Li, Hong Hao. *Development of efficient methods for prediction of medium to large scale BLEVE pressure in open space*. Pages 421-435.

The current practice in predicting the Boiling Liquid Expanding Vapour Explosion (BLEVE) pressure for structural response analysis and design is based mainly on some semi-empirical energy equivalency methods. These methods are relatively easy to use but may not give accurate BLEVE pressure predictions. Using numerical simulations can yield better BLEVE pressure predictions, but it requires profound modelling knowledge and is time-consuming, which may not be viable to many design and consulting offices. This study generates empirical formulae and charts for easy and accurate predictions of BLEVE pressure using in the analysis and design of structures against BLEVE loads. The empirical relations of critical parameters, namely the side-on peak pressure, peak pressure rise time, duration, arrival time and impulse that are needed to fully define the pressure-time history, as functions of BLEVE parameters are established. The performances of the proposed empirical formulae and charts are evaluated by comparing the prediction results with experimental data. It is proven that the developed BLEVE pressure prediction equations and charts are easy to use and yield more accurate BLEVE pressure predictions than other commonly used empirical methods.

- **Keywords:** BLEVE; Pressure-time history; BLEVE energy; BLEVE pressure prediction equations; BLEVE pressure prediction charts

Jaewon Lee, Sunghyun Cho, Hyungtae Cho, Seungsik Cho, Inkyu Lee, Il Moon, Junghwan Kim. *CFD modeling on natural and forced ventilation during hydrogen leaks in a pressure regulator process of a residential area*. Pages 436-446.

Hydrogen fuel cells have been installed in more than 100 facilities and numerous homes in Ulsan hydrogen town in the Republic of Korea. Despite the advantages of hydrogen,

accidents can still occur near residential areas. Thus, appropriate risk mitigation plans should be established. In this study, a computational fluid dynamics (CFD) model of natural and forced ventilation is presented as an emergency response to hydrogen leakages in pressure regulator equipment housing. The CFD model is developed and investigated using three vent configurations: UP, CROSS, and UP-DOWN. The simulation results indicate that the UP-DOWN configuration achieves the lowest internal hydrogen concentration out of the three. In addition, the relationship between the total vent size and internal hydrogen concentration is determined. A vent size of 12% of the floor area has the lowest hydrogen concentration. The use of nitrogen for forced ventilation during emergencies is proposed to ensure that the hydrogen concentration of the released gas is less than one-fourth of the lower flammability limit of hydrogen. Compared to natural ventilation, the time required to reach safe conditions is decreased when nitrogen forced ventilation is used.

- **Keywords:** Computational fluid dynamics; Hydrogen safety; Hydrogen leakage; Natural ventilation; Nitrogen forced ventilation

Huiming Sun, Song Guo, Sining Chen, Min Jia, Shuyi Shen. *Thermal behavior and decomposition mechanism of azobenzene by using kinetic calculation method and molecular dynamics simulation method*. Pages 447-453.

In the work, both elevated thermal and isothermal experiments of azobenzene were carried out by using SENSYS Evolution DSC. Kinetic parameters and decomposition mechanism were figured out by using Kinetic Calculation (KC) method and Molecular Dynamics Simulation (MDS) method. The results show that a first endothermic and following exothermic behavior appears distinctly in the thermal decomposition process of azobenzene; the apparent activation energy keeps approximately constant at the stage of $0.1 \leq \alpha \leq 0.4$, and then reduces gradually as the reaction goes on; the thermal decomposition behavior of azobenzene can be described by Sestak-Berggren mechanism on here; The step without adequate free radicals and the step with exponential growth of free radicals dominate respectively the stable decomposition process at initial stage and the self-accelerating decomposition process at autocatalytic stage; Based on Semenov model, the calculated SADT of azobenzene is 380.5 ℃, when packed in 25 kg standard package.

- **Keywords:** Azobenzene; Thermal kinetics; Decomposition mechanism; Thermal hazard; Molecular dynamics simulation

Yong Wang, Yan Wang, Yangxian Liu. *Oxidative removal of gaseous hydrogen sulfide by a dual ions-dual oxidants coupling activation system*. Pages 454-465.

A gaseous hydrogen sulfide (H2S) oxidative removal technology by a dual ions-dual oxidants coupling activation system (i.e., Cu2+/Fe2+/persulfate(PS)/H2O2 coactivation system) was put forward. The fundamental issues, mainly including H2S removal performance, process parameters optimization, products, free radicals, synergy mechanism and desulfurization mechanism were studied systematically in a bubble column reactor. The study indicates that compared with Fenton system and non-coupling activation systems, the new dual ions-dual oxidants coupling coactivation system shows much higher free radical yield and H2S removal efficiency owing to significant synergistic activation effect. Higher concentrations of Cu2+ or Fe2+ greatly increase the H2S removal efficiency. With the increase of PS concentration, H2O2 concentration or reagent pH value, the H2S removal efficiency is first enhanced, and afterwards slightly declined. The H2S removal efficiency is declined via increasing operating temperature, gas flow rate and contents of H2S, SO2, NO and CO, and is almost not affected by content of Hg0.

Sulfate, CuS and elemental sulfur are determined to be the products of H2S removal, and no by-products are produced after the reaction. Oxidation via ·OH and SO4-· plays a crucial role in H2S removal, which is proved to be the primary pathways of H2S removal. Finally, the recovery strategy of the products is discussed preliminarily.

- **Keywords:** Hydrogen sulfide; Advanced oxidation; Dual ions-dual oxidants; Coupling activation; Bubble column reactor

Shangding Yang, Liuyang He, Pai Peng, Yanli Liu, Yongfei Ma, Li Wu, Zulin Zhang, Lie Yang. *Synergistic Fe2+/UV activated peroxydisulfate as an efficient method for the degradation of thiacloprid*. Pages 466-475.

Increasing usage and emission of neonicotinoid insecticides have caused severe risks to ecological environment and human health. The study aimed to explore a Fe2+/UV/ peroxydisulfate (PDS) system for effective degradation of thiacloprid (TCP). The effects of various parameters involving the degradation efficiency including initial solution pH, PDS concentration, Fe2+ concentration, and UV power were investigated. Under the optimized conditions (pH 3.0, PDS concentration of 1 mmol L−1, Fe2+ concentration of 0.36 mmol L−1, and UV power of 45 W), it was observed that 97.5% of TCP was degraded with a pseudo-first-order kinetics reaction constant of 5.63 × 10−2 min−1. The Fe2+/UV/PDS system demonstrated excellent performance on reaction stoichiometry efficiency (RSE) (31.25%, 60 min). Meanwhile, the effects of inorganic anions (Cl-, NO3- and HCO3-) and natural organic matter (humic acid) on the removal of TCP were also investigated. In addition, the free radical scavenging experiments indicated that SO4•- was dominant in the Fe2+/UV/PDS system. The intermediates were identified and their toxicity was notably lower than that of TCP. Therefore, the Fe2+/UV/PDS system is efficient and ecologically safe for TCP removal from wastewater.

- **Keywords:** Peroxydisulfate; Ferrous iron; Ultraviolet; Thiacloprid; Natural anions

Wenhe Wang, Sen He, Tengfei He, Tianyu You, Trent Parker, Qingsheng Wang. *Suppression behavior of water mist containing compound additives on lithium-ion batteries fire*. Pages 476-487.

In this work, a new type of compound additive and water mist compatible fire extinguishing method was designed, and the effects of its suppression on a 18650 LiMn2O4/Li(Ni0.5Co0.2Mn0.3)O2 lithium-ion battery fire was investigated. To do so, a self-designed experimental platform was used to study the fire extinguishing capabilities and influence of the composite additives containing water mist on a lithium-ion battery fire. Several cell parameters were measured to evaluate the suppression effect of the fire extinguishing method, such as extinguishing time, maximum temperature, and heat release rate. The results show that both physical and chemical additives can play significant physicochemical roles in extinguishing fires and are more effective than pure water mist. The physical additives enhance the heat absorption and cooling as well as radiation heat barrier and oxygen asphyxiation mechanisms by reducing the surface tension and droplet size in the fog field. Furthermore, the chemical additives enhance the fire extinguishing efficiency by decomposing the active gases CO2 and H2O in the fire field and capturing the free radicals of the flame in the battery combustion reaction.

- **Keywords:** Lithium-ion batteries; Fire; Water mist; Additives; Suppression mechanism

Rongxing Bian, Tingxue Zhang, Fengbin Zhao, Jihong Chen, Chenyu Liang, Weihua Li, Yingjie Sun, Xiaoli Chai, Xin Fang, Liqun Yuan. *Greenhouse gas emissions from waste sectors in China during 2006–2019: Implications for carbon mitigation*. Pages 488-497.

Reducing carbon emissions has been the consensus among countries worldwide. As an important anthropogenic source of greenhouse gas (GHG), however, the GHG emission pattern from the waste sector in China's cities and counties is unclear which hinders the development of an effective strategy for GHG reduction. In this study, the GHG emissions from the waste sector of China during 2006–2019 were studied based on the Intergovernmental Panel on Climate Change (IPCC) inventory models. The total GHG emissions from the waste sector increased from less than 55.38 million metric tons (Mt) in 2006–178.06 Mt in 2019, with landfills accounting for the majority of GHG emissions. The proportion of GHG emissions from municipal solid waste (MSW) incineration increased rapidly from 7.8% in 2006 to 22.4% in 2019. The GHG emissions increased rapidly from less than 2.67 Tg in 2006–55.64 Mt in 2019, with the contribution increasing from 4.8% to 31.2%, as more MSW was landfilled. Among the seven regions of China, Eastern China contributed the most to GHG emissions. Therefore, there is a significant GHG mitigation potential in the MSW disposal sector. These findings indicate that GHG mitigation strategies should be based on the MSW generation and disposal situation, economic level, and operational management level of each region and province.

- **Keywords:** GHG emission inventory; Waste sector; China; Reduction potential

Tarsila F. de Castro, Daniela V. Cortez, Daniel B. Gonçalves, Heitor B.S. Bento, Rhyan L.N. Gonçalves, Tales A. Costa-Silva, Bruno C. Gambarato, Heizir F. de Castro, Ana Karine F. de Carvalho. *Biotechnological valorization of mycelium-bound lipase of Penicillium purpurogenum in hydrolysis of high content lauric acid vegetable oils*. Pages 498-505.

The study deals with the direct use of whole cells of a species of Penicillium as biocatalyst (mycelium-bound lipase) for the hydrolysis of vegetable oils under low-power ultrasonic irradiation. Whole cells of Penicillium purpurogenum with lauric acid-specificity lipase were able to hydrolyze vegetable oils with high content of this fatty acid. Up to 90% hydrolysis values were reached at 7 h of reaction, providing high fatty acid contents in shorter times concerning the literature. The results suggest that the ultrasound wave improves the interfacial area and that the lipase of Penicillium purpurogenum is bound to the cell, in a place with easy access to the substrate. On the other hand, the presence in the substrate of fatty acids with 18 carbons (stearic, oleic, and linoleic) in a concentration greater than 20%, negatively interferes with the degree of hydrolysis, indicating a possible limitation of lipase specificity. The present study highlights the biotechnological potential of mycelium-bound lipase (naturally immobilized enzymes) for use in the hydrolysis of babassu, coconut and kernel oils, which are not directly integrated into the food production chain.

- **Keywords:** Biomass valorization; Penicillium purpurogenum; Mycelium-bound lipase; Hydrolysis; Lauric acid

Zhonghua Sheng, Guogang Yang, Shian Li, Qiuwan Shen, Han Sun, Ziheng Jiang, Jiadong Liao, Hao Wang. *Modeling of turbulent deflagration behaviors of premixed hydrogen-air in closed space with obstacles*. Pages 506-519.

The propagation of premixed hydrogen-air deflagration flames in a closed duct with different shapes of obstacles was investigated using large eddy simulation (LES). The turbulent flame wrinkling factor in the LES subgrid turbulent combustion model is

dynamically modeled based on Charlette's power-law model. The LES results obtained by the dynamic flame surface density (DFSD) model can accurately match the experimental data quantitatively and qualitatively. Numerical results show that the triangular obstacle induces a higher peak overpressure, 7% and 30% higher than that in the square and circle, respectively. The formation of juxtaposed tulip flames is discovered, and the topological analysis of the velocity vector field reveals that the vortex at the tail of the obstacle is the main inducing factor for its formation. Additionally, the Karlovitz number is used to quantify the degree of turbulence-flame interaction, and the transition of deflagration flame from "wrinkled flame" to "thin reaction zone" is observed. The research helps to understand the mechanism of deflagration flame propagation induced by obstacles and provides critical information for safety planning and explosion protection.

- **Keywords:** Large eddy simulation; Dynamically modeled; Closed space; Obstacle shape; Juxtaposed tulip flames

Edvinas Krugly, Oleh Pitak, Darius Ciuzas, Martynas Tichonovas, Inga Stasiulaitiene, Tadas Prasauskas, Linas Kliucininkas, Dainius Martuzevicius. Removal of VOCs from wood processing ventilation air by advanced oxidation gas-to-particle prototype system. Pages 520-527.

Industrial gaseous emissions of volatile organic compounds (VOCs) may result in adverse effects to environment and human health, thus must be removed from flue gas before emitted to the atmosphere. Here we present a study of a real-world testing of a novel hybrid gas-to-particle conversion system targeting VOC removal from the ventilation air originating at wood processing facilities. Terpenes (primarily α-pinene, β-pinene, and α-terpineol) were targeted as the prevailing VOCs. The system was realized as a single-pass reactor having multiple stages of plasmolysis/ozonolysis, photolysis, nucleation, coagulation and agglomeration of aerosols, as well as precipitation of agglomerates in an electrostatic field. The VOC removal efficiency in terms of total VOCs (TVOCs) has reached 92.8%, while 100% removal efficiency of α-pinene, β-pinene, and α-terpineol was achieved with the non-thermal plasma (NTP) operating at a specific energy input (SEI) of 3.6 J/L (42 J/L of entire system). The advanced gas-phase oxidation system proved to be competitive in treating VOC polluted flue gases in terms of removal efficiency and relatively low energy input. The results hereafter promote faster development and extensive industrial application of gas-phase advanced oxidations systems based on the gas-to-particle conversion process.

- **Keywords:** Gas-phase advanced oxidation; Gas-to-particle conversion; VOC emission treatment; Wood drying emissions

Min Huang, Guohua Chen, Peng Yang, Kun Hu, Lixing Zhou, Jinkun Men, Jie Zhao. *Multi-hazard coupling vulnerability analysis for buckling failure of vertical storage tank: Floods and hurricanes*. Pages 528-541.

As one of the typical multi-hazard natural disasters, floods and hurricanes have caused destructive damage to the process equipment, especially vertical storage tanks, leading to a large number of severe technological accidents in chemical industrial parks. In the present study, aiming at the buckling behavior under the coupling effect of floods and hurricanes, the wind load, flood load, and wave load are analyzed, and the limit state equation of storage tank buckling failure under the coupling effect of floods and hurricanes is established. Then, the load distribution on the tank wall is verified by FLUENT software and the rationality of FLUENT simulation is shown by laboratory experiments of vertical storage tanks. The fragility curves and surfaces are plotted by Monte Carlo Simulation under different wind speeds, considering the effects of flood velocity, flood inundation height, and liquid filling level. The results show that with the

increase of wind speed, the influence of flood inundation height on the vulnerability of storage tanks gradually increases, while the influence of flood velocity and filling level on the vulnerability of storage tanks gradually decreases. Flood inundation height is the main disaster parameter affecting the vulnerability of storage tanks. Compared with the case of floods or hurricanes alone, the buckling failure probability of storage tanks under the coupling effects of floods and hurricanes increases by 17.67% and 80.50%, respectively. Moreover, the damaging effect of the coupling of floods and hurricanes is greater than that of the direct superposition effect, and the failure probability increases by 17.57%. The research aims to analyze the failure mechanism of vertical storage tanks, accident prevention, and control under the coupling effects of multiple hazards.

- **Keywords:** Flood; Hurricane; Coupling effect; Limit state equation; Vulnerability

Xiaoyun Dai, Chengyuan Su, Zhuxin Chen, Xinjuan Li, Pingping Lu, Zhifei Qi, Zehua Luo, Menglin Chen. *Sulfonamide and quinolone antibiotics contaminated wastewater treatment by constructed rapid infiltration: efficiency and microbial community structure*. Pages 542-555.

Four antibiotics common in wastewater, namely sulfadiazine (SD), sulfamethoxazole (SMX), ciprofloxacin (CIP), and norfloxacin (NOR), were used in the treatment of wastewater by constructed rapid infiltration (CRI), using coke as filler material. Results showed that the removal rates of chemical oxygen demand (COD), ammonia nitrogen (NH3-N) and the total phosphorus (TP) of the sulfonamide antibiotics infiltration column reached 75.01%, 40.79% and 91.22%, respectively, which were 6.61%, 12.13% and 2.68% lower than those of the quinolone antibiotics infiltration column. With increasing antibiotic concentration (2–10 mg/L), the removal of SD showed a downward trend. The average removal rates of CIP and NOR by the CRI reached 34.65% and 43.57%, respectively. Oxygen-containing functional groups of the coke played a positive role in the removal of antibiotics. The dehydrogenase (DH) activity in the sulfonamide infiltration column was 0.62 μg/(g·mL), which was 0.48 μg/(g·mL) lower than that of the quinolone infiltration column. Meanwhile, the activity of phosphatase (AKP) in the sulfonamide infiltration column was 0.06 mg/(g·h), 0.30 mg/(g·h) lower compared to that of the quinolone infiltration column. Microbial community was dominated by Actinomycetes (38.52–55.93%) at the phylum level and by Arthrobacter (34.00–49.20%) at the genus level, especially in the sulfonamide infiltration column. Based on Kyoto Encyclopedia of Genes and Genomes (KEGG) functional analysis, carbohydrate (10.79–11.52%) and amino acid metabolism (10.79–11.27%) were the main bacterial pathways. Overall, sulfonamide antibiotics more negative impacted wastewater treatment by the CRI than quinolone antibiotics.

- **Keywords:** Antibiotic wastewater; Constructed rapid infiltration; Coke; Microbial community structure; KEGG

Jeny Elihut Ventura Gutiérrez, Franciele Pereira Camargo, Isabel Kimiko Sakamoto, Maria Bernadete Amâncio Varesche. *Expanded granular sludge bed reactor technology feasibility for removal of nonylphenol ethoxylate in co-digestion of domestic sewage and commercial laundry wastewater: Taxonomic characterization and biogas production*. Pages 556-570.

Nonylphenol Ethoxylate (NPEO) is a non-ionic surfactant used worldwide in the formulation of cleaning products. Removal of these compounds from domestic sewage is difficult to achieve. In this study, the degradation of NPEO from the co-digestion of domestic sewage (DS) and commercial laundry wastewater (CLW) was evaluated using a pilot-scale expanded granular sludge bed (EGSB) reactor operated for 637 days. In phase

I, the reactor was fed with synthetic substrate (SS) – without NPEO, phases II and III with SS plus 3.5 ± 1.0 mgNPEO L−1 and 7.6 ± 2.1 mgNPEO L−1, respectively. Phase IV with SS plus CLW containing 4.0 ± 1.1 mgNPEO L−1, phase V with DS plus CLW and 3.7 ± 1.3 mgNPEO L−1. Nearly 60% of NPEO was biodegraded and chemical oxygen demand (COD) removal varied from 90 ± 5% to 97 ± 2% (for up to 573.8 ± 130.1 mgCOD L−1). Spirochaetacea exhibit the greatest relative abundance (from 65.3% to 90.7%) throughout the operation. NPEO addition negatively affected methanogenic activity, such that CH4 yield decreased 91% even at high COD removal. Surprisingly, after 549 days of operation, a CH4 yield of 0.30 ± 0.14 LCH4 gCOD−1 removed was observed.

- **Keywords:** Emerging contaminants; NPEO biodegradation; Anaerobic co-digestion; Spirochaetacea; Methane yield

Ahmad Muzammil Idris, Risza Rusli, Mohammad Shakir Nasif, Ahmad Fakrul Ramli, Jeng Shiun Lim. *A fuzzy multi-objective optimisation model of risk-based gas detector placement methodology for explosion protection in oil and gas facilities*. Pages 571-582.

A flammable gas detection system is one of the critical control strategies of catastrophic events such as fire and explosion. While gas detector technology has improved significantly, adopting a methodology for optimal placement of gas detectors is still an issue, especially when integrated with a risk-based approach. An enhancement of a risk-based approach is proposed to optimise the placement of flammable gas detectors by integrating a formulation of fuzzy multi-objective mixed-integer linear programming with the goal of minimising the residual risk and total number of detectors for effective explosion protection. The proposed methodology primarily begins with the identification of critical leak scenarios that require detection followed by the prediction of a targeted gas cloud and dispersion analysis using a computational fluid dynamic model. Risk analysis is conducted to identify high risk areas that need flammable gas detectors protection, which is the input for the mathematical model. The proposed risk-based model was tested using a case study involving a natural gas liquids (NGL) recovery unit, and the results were compared to a published greedy algorithm (GA) formulation. By using mixed-integer linear programming (MILP) formulation, the number of detectors needed are lower with higher risk reductions compared to the GA formulation. Additionally, a sensitivity analysis was performed to determine the proposed model's response to parameter variations.

- **Keywords:** Gas detectors optimisation; Fuzzy multi-objective; Explosion; Risk-based; Computational fluid dynamics

Kai Wang, Mingqing Su, Lijun Wei, Sining Chen, Xiangbei Kong, Yunlong Fang. *Effect of initial turbulence on explosion behavior of stoichiometric methane-ethylene-air mixtures in confined space*. Pages 583-593.

The turbulent explosion process of stoichiometric CH4/C2H4/air mixtures was experimentally studied by using a standard 20 L sphere explosion system and it's powder storage tank as the turbulence generator. Taking the initial turbulent environment and ethylene volume fraction as variables, the effects of turbulence intensity and fuel composition on explosion characteristics were studied. The results show that both turbulence intensity and ethylene content promote the explosion of the mixtures and increase the severity of the explosion, but the influence of turbulence intensity on combustion evolution mainly focuses on heat loss, while the influence of ethylene content mainly focuses on adiabatic explosion. When the ethylene ratios increase to 0.5 or more, the increase of explosion severity caused by turbulence is not obvious. The analysis of experimental results and numerical simulation shows that the influence of initial

turbulence generated by powder storage tank on explosion is the result of the combined action of turbulent kinetic energy and combustible gas redistribution.

- **Keywords:** Methane/ethylene; Explosion characteristic; Combustion time; Heat loss; Turbulence influence

Gongduan Fan, Junkai Zhang, Yingmu Wang, Keshu Huang, Shumin Wang, Yixin Yao, Jing Luo. *Microbial community and nitrogen transformation pathway in bioretention system for stormwater treatment in response to formulated soil medium*. Pages 594-602.

Bioretention system has been commonly recognized as an emerging management method to control urban rainwater runoff. However, nitrogen conversion mechanisms in bioretention system in response to formulated soil medium remains unknown. In this work, five bioretention columns with different formulated soil medium were established, and results indicated that all bioretention columns achieved high NH4+-N removal rate, but exhibited significantly different NO3--N removal performance. High-throughput sequencing results suggested that nitrification might be achieved by heterotrophic nitrifying bacteria, while Pseudomonas and Rubellimicrobium may be the main denitrifying bacteria, which served as anaerobic and aerobic denitrifier, respectively. Heterotrophic nitrification-anaerobic/aerobic denitrification may the microbial pathways to realize effective nitrogen removal performance in these bioretention systems. Bioretention system with moderate silt content (NC, 10%) displayed higher abundant potential denitrifier, leading to better nitrogen removal performance. Besides, soil adsorption played an important role in nitrogen removal, particularly when activated carbon was added. This work could provide guidance of formulated soil medium optimization for the application of bioretention systems.

- **Keywords:** Bioretention system; Rainwater management; Formulated soil medium; Nitrogen transformation; Microbial community

Erguang Huo, Liyong Xin, Shijie Zhang, Chao Liu, Shukun Wang, Lu Zhang. *The combustion mechanism of leaking propane (R290) in O2 and O2/H2O environments: ReaxFF molecular dynamics and density functional theory study*. Pages 603-610.

Propane (R290) is a widely used environmentally friendly refrigerant with excellent thermodynamic properties, but it may burn once it leaks. Therefore, it is imperative to investigate the combustion mechanism of leaking propane. A series of ReaxFF molecular dynamic simulations were employed, and the reactions involving the decomposition of propane were investigated by density functional theory (DFT), and the results of the ReaxFF molecular dynamic simulations were clarified by comparing the energy barriers, bond dissociation energies and reaction energies required for the reactions. The results indicated that the chemical role of H2O was mainly reflected by the reactions of H2O molecules with H and O radicals to form OH radicals and H2 molecules. The combustion of propane was promoted by the presence of a low concentration of H2O molecules.

- **Keywords:** ReaxFF; Density functional theory; Combustion mechanism; Propane (R290); H2O

Yong Sun, Zhen Qin, Yuting Tang, Chengfeng Liao, Yuchen Liu, Xiaoqian Ma. *Techno-environmental-economic assessment on municipal solid waste to methanol coupling with/without solid oxygen electrolysis cell unit*. Pages 611-628.

Integrating municipal solid waste (MSW) gasification with renewable energy to synthesize methanol shows great potential in alleviating the dependence on fossil energy and reducing the negative environmental impact of increasing MSW production. In this study, three technological processes including MSW-to-methanol integrated with carbon capture and storage (MTMC), MSW-to-methanol integrated with solid oxygen electrolysis cell unit (MTMS) and MSW incineration to power (MTP) are compared from the perspective of techno-environmental-economic performance. Results show that MTMS process owns the maximum exergy efficiency (60.8%), followed by MTMC (41.5%) and MTP (18.9%). In terms of global warming potential (GWP), MTP process has the worst environmental performance with 19,164.84 kgCO2eq/h. The economic analysis shows that MTMS process owns the highest value of levelized profit of MSW (LPOM) with 38.64 USD/t under the current market conditions. In addition, comparative analysis shows the production cost of methanol (PCOM) of MTMC and MTMS routes is 406.09 USD/t and 355.89 USD/t, respectively, which are economically competitive compared with the coal / biomass / CO2 hydrogenation to methanol route. Sensitivity analysis shows that MTMS process processes its advantage on economic performance only if the methanol price is higher than 350 USD/t and photovoltaic on-grid tariff is lower than 0.055 USD/kWh.

- **Keywords:** Municipal solid waste; Gasification; Solid oxygen electrolysis cell; Techno-environmental-economic assessment; Recycling

Bo Li, Run Huang, Renqi Xie, Qinghui Wu, Anxun Xu. *A novel process for the direct utilization of copper slag and phosphate rock by compound modification and coreduction*. Pages 629-639.

The traditional direct reduction–separation approach used to economically and effectively treat copper slag (CS) or phosphate rock (PR) encounters challenges, such as low metal recovery, high cost, and high additive requirements. In this paper, an ecofriendly process for synchronously utilizing CS and PR by compound modification and coreduction, accompanied by magnetic separation, is proposed to resolve these limitations. In this approach, use graphite as a reductant toreduce Fe and the CaO in the PR catalyzed the reduction of fayalite in the CS, thereby enhancing Fe formation. Owing to its low melting point, CS generated a liquid phase and improved the growth of particles, which was beneficial for producing ferrophosporus (Fe–P) alloys. The Fe–P and slag were separated and recovered, owing to their melting point and density differences, thereby highlighting the efficiency of the proposed method. After comprehensive consideration, a crude Fe–P alloy containing 82.31% Fe and 13.65% P was prepared under optimal conditions and suitable for the production of battery grade iron phosphate.

- **Keywords:** Copper slag; Phosphate rock; Compound modification; Coreduction; Fe–P alloy

Zhenxiang Feng, Yonggang Li, Bing Xiao, Bei Sun, Chunhua Yang. *Process monitoring of abnormal working conditions in the zinc roasting process with an ALD-based LOF-PCA method*. Pages 640-650.

Timely and accurate detection of abnormal working conditions can ensure stability, improve production efficiency and reduce pollution of an industrial process. However, the production data of an industrial process has non-Gaussian and time-varying characteristics due to the diverse feed composition and complex reaction mechanisms. To address the above issue, an improved online principal component analysis (PCA)

algorithm based on the selective model update is proposed in this study. First, considering the non-Gaussian nature of the process data, a local outlier factor-based (LOF) abnormality detection logic is used to replace the T2 and squared prediction error (SPE) statistics in traditional PCA algorithms. Then, to adapt to the time-varying characteristics of the process data, an approximate linear dependence (ALD) algorithm is used to evaluate the independent degree between the new sample and training samples. Only those samples containing new information are used to update the monitoring model, which can improve model performance and reduce the frequency of online updates. The zinc roasting process (ZRP) is used as an example to illustrate the proposed approach. Industrial data collected from a ZRP is used to demonstrate the performance of the ALD-based LOF-PCA method in the early detection of two typical abnormal working conditions in the ZRP.

- **Keywords:** Zinc roasting process; Abnormal working conditions; Process monitoring; Local outlier factor-principal component analysis (LOF-PCA); Approximate linear dependence

Jiliang Liu, Zhonghua Wang, Guangsheng Li, Yongying Jia, Chuan Ma, Haiqian Zhao, Xiaoyan Liu. *Recognition of the effect of O2 on the complexation absorption of NO in the FeII/Na2SO3 system*. Pages 651-657.

The presence of O2 in a FeII/Na2SO3 system severely affects its denitrification efficiency. In this study, the influence of O2 on NO absorption via complexation was studied in terms of three aspects: direct oxidation of NO, consumption of complexation reactants, and advanced oxidation processes. Experimental results showed that under the experimental conditions, the existence of O2 exerted different effects on different stages of NO absorption. In the first 5 min of the reaction, the increased O2 concentration promoted the denitrification efficiency of the FeII/Na2SO3 system. After 5 min, the inhibition increased. The direct oxidation of NO using O2 improved the denitrification efficiency in the initial stages of the reaction. However, this effect was minimal and the maximum oxidation rate was only 14.88% under 8% O2. The rapid oxidation of FeII and SO32- using O2 induced their direct rapid consumption of FeII and SO32- in the system, which was the main reason in the reduction of the denitrification efficiency. O2 caused advanced oxidation processes, but these processes generally reduced the denitrification efficiency.

- **Keywords:** Advanced oxidation processes; Denitrification; FeII/Na2SO3 system; Influence; O2

Jian Gao, Chunqiang Lu, Wei Su, Zhiqiang Li, Xingyun Li, Yannan Zhao, Guixian Deng, Kongzhai Li. *Exploring the effect of calcination temperature and sulphuric acid impregnation treatment on the NH3-SCR activity of cold-rolled sludge*. Pages 658-668.

In recent years, sulphate materials have received more and more attention because of high activity in the selective catalytic reduction of nitrogen oxides with ammonia (NH3-SCR). In this paper, a series of catalysts for NH3-SCR were prepared by sulphuric acid impregnation and calcination at different temperatures of cold-rolled sludge which main component is iron oxide. The performance of cold-rolled sludge catalyst was measured by X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM), temperature programmed-reduction of hydrogen (H2-TPR), temperature programmed desorption of ammonia (NH3-TPD) and X-ray photoelectron spectroscopy (XPS). It was demonstrated that the increase of iron sulphate and Fe3+ content can be observed in the cold-rolled sludge after sulfuric acid impregnation and low temperature calcination (300 ℃), which leads to the improvement of SCR denitration performance. The results

show that 100% denitration conversion can be achieved at 280 °C via the modified cold-rolled sludge, with 94% of the performance was retained after the introduction of SO2 and H2O for 5 h. There are minor morphological structural changes in the catalyst, while the redox properties and acidity of the catalyst changed significantly after the treatment process of sulfuric acid impregnation and calcination. This means that the enhanced redox properties and acidity of the catalyst play a key role in improving the activity of NH3-SCR.

- **Keywords:** NOx; Sulfate catalyst; NH3-SCR; Industrial waste-derived catalysts; SO2-tolerance

Haosheng Sun, Jun Qin, Ludong Yi, Yinghao Ruan, Jun Wang, Dawei Fang. *A new process for degradation of Auramine O dye and heat generation based on orifice plate hydrodynamic cavitation (HC): Parameter optimization and performance analyses*. Pages 669-683.

Hydrodynamic cavitation (HC) is not only a promising wastewater treatment technology but also an efficient heat generation method. In this work, the HC degradation of several organic dyes was carried out and the related heat generation was studied. The effects of geometrical parameters (orifice angles (α = 0 ° and± 45 °) and orifice numbers (n = 3–9)) and experimental parameters (2.0–4.0 bar pressures, 30–60 °C temperatures and 5.0–15 mg/L concentrations) on Auramine O degradation and heat generation in orifice plate HC system are investigated. TOC analysis is performed to determine the mineralization degree of Auramine O solution. The generated intermediates are detected by LC-MS. In addition, the produced free radicals in HC process are identified by adding some trapping agents. The results showed that the HC technology has high mineralization and strong heat generation abilities in degradation processes of organic pollutants. For 6-orifice plate, 4.0 bar pressure, 5.0 L solution volume and 10 mg/L concentration, 81.39% degradation ratio of AO was achieved at 90 min cycle moment. And that, 1082.52 kJ heat energy with 40.09% thermal efficiency was obtained during 30 min cycle time. Perhaps, this work may provide a new strategy for simultaneous large-scale organic wastewater treatment and effective heat production recycle.

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

Bharti Saini, Manish Kumar Sinha, Anirban Dey. *Functionalized polymeric smart membrane for remediation of emerging environmental contaminants from industrial sources: Synthesis, characterization and potential applications*. Pages 684-702.

Polymeric membrane technology has been accepted as one of the significant tools in separation and purification process. Membrane preparation, modification and characterization are the key steps for selection of membrane in a specific applications. This review work may offer a point of reference to the researchers who are concern in fabrication of polymeric membrane via phase inversion method dedicated on immersion precipitation. In this review article, special consideration has been paid to the evaluation of polymeric membrane properties such as casting solution viscosity, coagulation value, membrane morphology, structure, chemical composition, porosity, shrinkage, hydrophilicity, water uptake, ion exchange capacity, pH-responsive behaviour, permeation, solute rejection, fouling behaviour and cleaning efficiency. This review article encompasses the applications of polymeric membrane in various fields.

- **Keywords:** Polymeric membrane; Phase inversion method; Membrane structure; Performance; Membrane applications

Parth Shah, Ashish Unnarkat, Femina Patel, Manan Shah, Parin Shah. *A comprehensive review on spinel based novel catalysts for visible light assisted dye degradation*. Pages 703-722.

Removal of color-causing compounds from wastewater is one of the major issues industries face because of its toxic, carcinogenic, baleful nature. It adversely affects aquatic life and human health too. Many processes are known to humankind, such as physiochemical, biological, chemical, and electrochemical. Advanced Oxidation Processes (AOPs) are of particular interest among these processes. The current review presents spinel-type photocatalysts for dye degradation that degrades the color-causing pollutants (dyes) and converts them into molecules such as CO2, H2O, and other simpler compounds depending on the structure of dyes. At first, the basics of photocatalyst degradation and its mechanism are discussed, followed by works with different catalyst spinels. The successive sections cover the effect of doping and parameters affecting photocatalysts. Three spinels: Nickel Ferrites, Cobalt Ferrites, and Zinc Ferrites are specifically discussed. Effects of doping on A sites and B sites are both reviewed. In general, doping alters the spinels' magnetic, optical, and structural parameters. Doping induces defects in the spinel lattice and thereby increases strain which causes oxygen vacancies and higher surface area with a reduction in particle or grain size, which finally results in better photocatalytic activity and ease of separation because of magnetic properties. The current work reviews the recent works carried out for photocatalytic dye degradation using spinel-type catalysts.

- **Keywords:** Novel catalyst; Dye; Visible light, Spinels; Photocatalysis; Dye degradation

Debashis Roy, Sudarsan Neogi, Sirshendu De. Degradative removal of Sulfamethoxazole through visible light driven peroxymonosulfate activation by direct Z-scheme MIL-53(Co/Fe)/MoS2 heterojunction composite: Role of dual redox mechanism and efficient charge separation. Pages 723-738.

MIL-53(Co/Fe)/MoS2 (MIL-MS) binary photocatalyst was synthesized by a hydrothermal procedure through insitu growth of MoS2 on MIL-53(Co/Fe). In comparison to pure MIL-53(Co/Fe) and MoS2, the binary catalyst having 10 wt% MoS2 (MIL-MS(10)) (0.01 g/L) achieved 99% Sulfamethoxazole (SMX) removal (10 mg/L) through visible light driven activation of peroxymonosulfate (PMS, 0.2 g/L), at initial solution pH of 6. The formation of heterojunction enhances the charge separation efficiency, activation of adsorbed PMS moieties and harvesting of incident visible light. Surface-bound Fe2+/Fe3+|surf., Co2+/Co3+|surf. and Mo4+/Mo6+|surf.redox perform significant roles towards charge transport and production of reactive species. EPR analysis, coupled with scavenging studies indicate that radical(SO4•−,O•H,O2•−,h+)involving oxidation mechanism imparted maximum contribution towards SMX degradation. Detailed degradation pathway was designed based on substantial intermediate analysis. Excellent visible light responsiveness, charge transfer ability and reusability over multiple catalytic cycles, coupled with excellent performance in various real water matrixes established MIL-MS composite as an ideal candidate for facile removal and mineralization of refractory organic contaminants under visible light irradiation.

- **Keywords:** Metal organic frameworks; MIL-53(Co/Fe); Heterojunction photocatalyst; Sulfamethoxazole; Peroxymonosulfate; Photocatalytic degradation

Ming Qiao, Ting Ren, Jon Roberts, Xiaohan Yang, Zhongbei Li, Jianming Wu. *New insight into proactive goaf inertisation for spontaneous combustion management and control*. Pages 739-757.

Spontaneous heating in the active goaf area during normal mining processes poses increased threats to mine productivity and safety, as evidenced in events induced by spontaneous combustion of coal. To control and mitigate this engineering problem, there is a need to gain critical knowledge of spontaneous combustion in the longwall goaf area, which can be achieved through a combination of field tests and numerical modeling. This paper introduces the spontaneous combustion management system widely used in Australia and presents Computational Fluid Dynamics (CFD) models for the simulation of gas flow dynamics in the goaf area, based on the site conditions of an underground coal mine where coal seam gas is predominantly comprised of carbon dioxide. The models were validated with gas monitoring data and used to conduct parametric studies for proactive goaf inertisation optimization. Qualitative and quantitative analysis of simulation results indicated that better goaf inertisation could be achieved when nitrogen was injected via cut-through at 250 m on the maingate (MG) side and surface boreholes at 100 m and 700 m on the tailgate (TG) side, with a total injection rate greater than 1750 l/s. The oxygen concentration on the MG and TG side dropped below 5% at distances of 120 m and 75 m behind the longwall face, with an oxidation zone area of 35375 m2, which was approximately one-third of the oxidation zone area of the scenario without inert gas injection. Simulation results help shed light on improving current goaf inertisation practices to effectively reduce the risk of heating in goaf areas and improve mining process safety based on Australian conditions and practices.

- **Keywords:** Spontaneous heating; Principal hazard management plan; Computational modeling; Proactive goaf inertisation; Inertisation parameter optimization; Mining process safety

Zahra Sakhaei, Masoud Riazi. *In-situ petroleum hydrocarbons contaminated soils remediation by polymer enhanced surfactant flushing: Mechanistic investigation*. Pages 758-770.

Chemicals injection for in-situ remediation of contaminated soils has attracted great attention. Efficiency of this technology relies on various parameters. Among them, chemical formulation of flushing agents has a key role. In this study, synergistic effect of Sodium Dodecyl Sulfate (SDS) ionic surfactant and Xanthan Gum (XG) biopolymer on the emulsification and solubilization of two types of petroleum hydrocarbon pollutants was investigated. Interfacial tension (IFT) measurements, bottle tests, droplet size distributions determination, and visual fluid flow experiments at pore-scale were conducted to assess pollutants removal strength of the proposed polymer enhanced surfactant flushing strategy. Results showed that although SDS surfactant reduced the equilibrium IFT of system to appropriate low value (i.e. less than 3 mN/m), it was not able to form stable oil-in-water emulsions. Nevertheless, addition of XG biopolymer, with no remarkable effect on IFT, improved emulsions formation and stability. Fluid flow experiments showed that oil snap-off and emulsion division are essential mechanisms of in-situ emulsion formation. A significant amount of hydrocarbon pollutants remained in porous medium after injection of 10 pore volumes of SDS. While, smaller size emulsions, as well as better contaminants removal were achieved for SDS solution with 4000 ppm XG at much lower injected pore volumes.

- **Keywords:** Environmental challenges; Petroleum hydrocarbons; Contaminated soils; Polymer enhanced surfactant (PES) flushing; Pore-scale mechanisms

Ujwal Shreenag Meda, Khushi Vora, Yash Athreya, Ujwal Arun Mandi. *Titanium dioxide based heterogeneous and heterojunction photocatalysts for pollution control applications in the construction industry*. Pages 771-787.

With increasing urbanization and industrialization there is an upsurge in air pollution that demands immediate attention. The use of nanomaterials to alleviate air pollution is gaining importance. Certain nanomaterials can photocatalytically act on air pollutants such as oxides of nitrogen (NOx), sulfur (SOx), and carbon (CO2), thereby bringing down their concentration locally. Titanium Dioxide (TiO2), its composites, and TiO2 based Z/S scheme heterojunction photocatalysts are a few such nanomaterials. The band-gap of TiO2 in solid-state (3.2 eV) makes it a good photocatalyst in the ultraviolet region and its composites in the visible light region of the spectrum. Metropolitan cities are densely filled with high-rise buildings and the exteriors of these buildings, which are largely exposed to the atmosphere, can be utilized to coat these nano materials to enable photocatalytic reduction of air pollutants in the surrounding atmosphere. The nano photocatalysts can either be applied as coatings on the existing buildings or incorporated into the construction materials during construction. In this review article, an attempt is made to cover the application of photocatalysts in the construction industry starting from the working principle (mechanism) of heterogeneous and heterojunction photocatalysts, their advantages and disadvantages, methods of synthesis, pollution control applications, with emphasis on the methods of incorporating the photocatalysts into construction materials and also as a coating on existing buildings, the set up required to evaluate NOx reduction and the factors that affect the NOx reduction. The current status of pollution control applications in the construction industry and the authors perspective on the application of heterojunction photocatalysts in construction industry are highlighted.

- **Keywords:** Degradation of air pollutants; Incorporation of nanoparticles into building materials; TiO2 based Z/S scheme photocatalysts; Nanocoatings; NOx reduction

Siraphatsorn Anusaraporn, Rujira Dolphen, Paitip Thiravetyan. *Importance of laccase enzyme and triiodide for gold leaching from silicate ore by marine bacterium Acinetobacter sp*. Pages 788-800.

The effect of enzymes and other substances on gold bioleaching was investigated. Acinetobacter sp. had a higher gold leaching performance than two strains of Vibrio sp. because it grew well in nutrient broth (NB) medium containing potassium iodide (KI) and produced high levels of both laccase and triiodide (I3-). Under two-step condition of Acinetobacter sp. in NB medium containing KI 10.9 g·L−1 and 1% (w/v) alkali lignin had the highest efficiency in gold leaching. Plausible mechanisms of gold bioleaching involved in biogenic iodide-iodine lixiviant and laccase reaction mechanisms. Laccase produced by Acinetobacter sp. could directly oxidize insoluble gold to soluble gold and also increase iodide oxidation. Afterward, the gold can be oxidized completely in the biogenic iodide-iodine lixiviant to form gold (I) diiodide [AuI2]- or gold (III) tetraiodide [AuI4]-. Interestingly, it was found that silicate ore could act as an inducer of laccase production. Furthermore, alkali lignin addition could increase gold bioleaching due to it can be used as a substrate for laccase production. Therefore, the two-step condition of Acinetobacter sp. could be applied in gold leaching under mild alkaline pH conditions. The advantage of this technology was safer and more environmentally friendly than cyanidation as a conventional extraction.

- **Keywords:** Bioleaching; Gold; Silicate ore; Acinetobacter sp.; Laccase; Triiodide

Abhinay Thakur, Savas Kaya, A.S. Abousalem, Shveta Sharma, Richika Ganjoo, Humira Assad, Ashish Kumar. *Computational and experimental studies on the corrosion inhibition performance of an aerial extract of Cnicus Benedictus weed on the acidic corrosion of mild steel*. Pages 801-818.

The corrosion inhibition investigation of aerial extract of Cnicus Benedictus, a weed referring to the Asteraceae family has been evaluated on the mild steel corrosion in 0.5 M HCl with the employment of the weight-loss method, potentiodynamic polarization measurements (PDP) and electrochemical impedance spectroscopy (EIS) techniques. This investigation demonstrated Cnicus Benedictus extract (CBE) as a green and sustainable mild steel corrosion inhibitor in 0.5 M HCl media exhibiting an inhibition efficacy of 92.45% at 1000 ppm. With the increased concentration of CBE, the value of icorr and corrosion rate (CR) decreased significantly from 7.4114 to 0.97438, revealing the protective effect of CBE on mild steel. The deposition of a highly defensive coating on the mild steel surface was demonstrated by the contact angle measurements. Additionally, the increase in the Kads values indicated a stronger interaction between the inhibitor molecules and metal surface. Furthermore, density functional theory (DFT) and Monte Carlo simulations have been utilized to validate the significant inhibition characteristic attained by the experimental study and to suggest an adsorption mechanism.

- **Keywords:** Cnicus Benedictus; Mild steel; Corrosion; Sustainable inhibitor; Adsorption; EIS; SEM

Hao Liu, Yajun Wang, Xiaohan Ren, Huanhuan Xu, Juan Chen. *Study on the transformation of Zn, Mn and Cr during sewage sludge combustion*. Pages 819-826.

Sewage sludge combustion experiments were carried out to investigate the migration and transformation of Zn, Mn, and Cr involved with the effects of combustion temperature, atmosphere, and steam concentration. The results showed that the volatilization of Zn was promoted by a temperature increase. Compared to air combustion, the inhibited volatilization of ZnCl2(g) and the production of ZnO promoted the recovery of Zn in ash during oxy-fuel combustion. Furthermore, the increasing temperature typically improved aluminosilicate capture MnO as well as the capability of CaO/Fe2O3 on capturing Cr. The reducing atmosphere caused by high CO2 concentration in oxy-fuel combustion facilitated the enrichment of Mn and Cr in ash. Steam favored the retention of Zn via transformation to form stable ZnO·A12O3·2SiO2 condensed into solid ash. The generation of CO and H2 from char-steam/char-CO2 gasification induced a local reducing atmosphere. It accelerated the transformation of MnO2 to MnO and facilitated the combination between MnO and aluminosilicate. Fe(III) reduced to Fe(II) strengthened the ability of iron oxide to capture Cr. The presence of steam promoted the decomposition of Ca-based minerals in the sewage sludge into a porous CaO, which enhanced the effect on Cr retention.

- **Keywords:** Sewage sludge; Heavy metals; Enrichment; Oxy-fuel combustion; Steam

Leila Feyzi, Nader Rahemi, Somaiyeh Allahyari. *Efficient degradation of tetracycline in aqueous solution using a coupled S-scheme ZnO/g-C3N4/zeolite P supported catalyst with water falling film plasma reactor*. Pages 827-847.

To overcome the plasma system drawbacks, the hybrid system is used for the removal of pharmaceutical pollutants from effluents. In this study, the tetracycline (TC) removal from water was investigated using hybrid water falling film plasma-catalyst system. The

ternary compounds nanocomposites containing zinc oxide (ZnO), nitride carbon graphite (g-C3N4), and zeolite with different ratios were synthesized at two stages using hydrothermal treatment method. Thereafter, the prepared nanocomposites were loaded on constructed plasma reactor equipped with the water falling film facility. The results of the characterization process confirmed that all synthesized nanocomposites had a suitable specific surface area, crystallinity, and the heterojunction formation ZnO with g-C3N4. The formation probability of S-scheme heterojunction structure of ZnO/g-C3N4 was discussed because of Fermi level's difference between ZnO and g-C3N4. Under the suitable operational condition, 95.5% TC removal efficiency as well as 4.43 synergistic effects were obtained using the hybrid system. The TC removal for hybrid system was ascribed as 30% more than sole plasma system. Afterward, the stability tests confirmed the ideal reusability of the prepared nanocomposite. The scavenger addition satisfied that the roles of both •OH and hole were critical. A mechanism was proposed for the TC degradation in this fabricated system.

- **Keywords:** Plasma; Falling film; ZnO/g-C3N4 catalyst; Synergistic effect; Tetracycline

Vinky Chow, Raphaël C.-W. Phan, Anh Cat Le Ngo, Ganesh Krishnasamy, Siang-Piao Chai. *Data-driven photocatalytic degradation activity prediction with Gaussian process*. Pages 848-859.

Photocatalysis has emerged as a powerful technology with beneficial impacts on the fields of science and engineering. To date, most photocatalysis research are experimentally-based that strongly rely on various experimental conditions. As the coronavirus pandemic hit the world in 2020, research and experiments were disrupted in various scientific disciplines. During these unprecedented times, machine learning plays a vital role in the continuity of photocatalysis research, notably for researchers under physical access restrictions. More specifically, machine learning is capable of predicting the photocatalytic efficiency and analysing the photocatalytic activity. In recent work, it was demonstrated that a Support Vector Regression (SVR) model succeeded in predicting the efficiency of methyl tert-butyl ether (MTBE) photodegradation using titanium dioxide (TiO2) as a photocatalyst, achieving a Root Mean Square Error (RMSE) of 5%. In this work, we investigate the applicability of the Gaussian Process (GP) technique to predict the photodegradation efficiency of contaminants catalyzed by pure and doped-titanium dioxide (TiO2); and we compare their performance with the current state-of-the-art SVR. Within this context, we discuss the foundations of both the machine learning models, as well as demonstrate how photocatalysis researchers can apply them to solving relevant problems in the field of photocatalysis.

- **Keywords:** Photocatalytic treatment; Photodegradation; Titanium dioxide; Machine learning; Gaussian process regression

Jinkun Men, Guohua Chen, Lixing Zhou, Peizhu Chen. *A pareto-based multi-objective network design approach for mitigating the risk of hazardous materials transportation*. Pages 860-875.

Hazardous materials (HazMat) transportation is one of the indispensable links in the chemical process industry and is closely related to safety, security, and environmental concerns. HazMat transportation routing is a major proactive risk management measure. Most related studies focus on diminishing the transportation risk for one single HazMat shipment. This work addresses a global perspective on the problem where the correlations of multiple simultaneous HazMat shipments are considered. A multi-objective transportation network design model is defined to optimize the objectives of the transportation risk and the transportation cost. A well-designed Pareto-based hybrid heuristic algorithm is proposed for model solving, which integrates a linear decomposition procedure for initial population construction, a Pareto-based scatter search procedure for

population evolution, and a variable neighborhood search procedure for solution improvement. Computational results indicate that the proposed algorithm is competitive in solving large-scale instances since it is able to strike a great balance between effectiveness and efficiency. The detailed solution analysis shows that the proposed approach can effectively coordinate multiple simultaneous HazMat transportation processes. Moreover, we find that performing multiple short-distance shipments would significantly reduce the total transportation risk, but results in the higher transportation cost. This work can provide a set of Pareto optimal transportation networks for different industrial application scenarios to achieve the trade-off between economic and safety.

- **Keywords:** Hazardous materials transportation; Chemical process industry; Proactive risk management; Transportation network design; Pareto optimal